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09/607142  
06/29/00

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

FILING UNDER 37 C.F.R. 1.53(b)

Box Patent Application  
Assistant Commissioner for Patents  
Washington, DC 20231

Express Mail Label No. EL 636738620US

Date of Deposit June 29, 2000

Sir:

This is a request for filing a divisional application under 37 C.F.R. 1.53(b) of  
Applicant(s): Cherry et al.

Title: Maltogenic Alpha-Amylase Variants

134 pages of specification 1 sheet of formal drawing

1 page of abstract

3 sheets of Executed Declaration and Power of Attorney

[x] The filing fee is calculated as follows:

|   |          |
|---|----------|
| Basic Fee:                                  | \$690.00 |
| Total Claims: $9 - 20 = 0 \times 18 =$      | \$0      |
| Independent Claims: $6 - 3 = 3 \times 78 =$ | \$234.00 |
| Total Fee:                                  | \$924.00 |

Priority of Danish application no. 98/00269 filed on February 27, 1998 is claimed under 35 U.S.C. 119. A certified copy was filed with U.S. Serial No. 09/386,607 filed on August 31, 1999.

Priority of U.S. provisional application no. 60/077,795 filed on March 12, 1998 is claimed under 35 U.S.C. 119.

The benefit of application no. PCT/DK99/00088 filed on February 26, 1999 in the PCT is claimed under 35 U.S.C. 120.

The benefit of application no. 09/386,607 filed on August 31, 1999 in the U.S. is

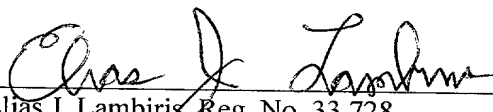
claimed under 35 U.S.C. 120.

Address all future communications to Steve T. Zelson, Esq., Novo Nordisk of North America, Inc., 405 Lexington Avenue, Suite 6400, New York, NY 10174-6401.

Please charge the required fee, estimated to be \$924, to Novo Nordisk of North America, Inc., Deposit Account No. 14-1447. A duplicate of this sheet is enclosed.

Respectfully submitted,

Date: June 29, 2000

  
Elias J. Lambiris, Reg. No. 33,728  
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**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE  
EXPRESS MAIL CERTIFICATE**

Box Patent Application  
Assistant Commissioner for Patents  
Washington, DC 20231

Re: U.S. Patent Application for  
Title: Maltogenic Alpha-Amylase Variants  
Applicants: Cherry et al.

Sir:

Express Mail Label No. EL 636738620US

Date of Deposit : June 29, 2000

I hereby certify that the following attached paper(s) or fee

1. Filing Under 37 C.F.R. 1.53(b) (in duplicate)
2. Patent Application (including 1 sheet of formal drawing)
3. Copy of Executed Combined Declaration and Power of Attorney
4. Preliminary Amendment
5. Information Disclosure Statement
6. Form PTO-1449
7. Request Transfer of Computer Readable Sequence Listing from Parent Case
8. Sequence Listing

are being deposited with the United States Postal Service "Express Mail Post Office to Addressee" under 37 C.F.R. 1.10 on the date indicated above and is addressed to the Commissioner of Patents and Trademarks, Washington, DC 20231.

Carol McFarlane

(Name of person mailing paper(s) or fee)

Carol McFarlane

(Signature of person mailing paper(s) or fee)

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**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Application of: Cherry et al.

Application No.: To be assigned

Group Art Unit: To be assigned

Filed: June 29, 2000

Examiner: To be assigned

For: Maltogenic Alpha-Amylase Variants

**PRELIMINARY AMENDMENT**

Assistant Commissioner for Patents  
Washington, DC 20231

Sir:

Before the above-captioned application is taken up for examination, entry of the following amendment is respectfully requested:

**IN THE SPECIFICATION:**

At page 1, after the title, insert

**--CROSS-REFERENCE TO RELATED APPLICATIONS**

This application is a divisional of U.S. application no. 09/386,607 filed on August 31, 1999, which is a continuation-in-part of PCT/DK99/00088 filed on February 26, 1999, and claims priority under 35 U.S.C. 119 of Danish application no. 98/00269 filed on February 27, 1998, and U.S. provisional application no. 60/077,795 filed on March 12, 1998, the contents of which are fully incorporated herein by reference.--

At page 3, line 30, insert the following:

**--BRIEF DESCRIPTION OF THE FIGURE**

Figure 1 shows the plasmid pLBei010, which contains the *Bacillus stearothermophilus* maltogenic amylase gene.--



At the top of page 49 (page 1 of the Appendix), insert the following heading:  
--Table 1 - Atom Coordinates from the Crystal Structure of NOVAMYL--.

**IN THE CLAIMS:**

Please cancel claims 10-34 without prejudice or disclaimer.

**REMARKS**

This amendment is submitted to cancel claims. Applicants submit that no new matter is added, and entry of the amendment is respectfully requested.

Respectfully submitted,

Date: June 29, 2000



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## MALTOGENIC ALPHA-AMYLASE VARIANTS

### FIELD OF THE INVENTION

The present invention relates to variants of maltogenic amylase and to methods of constructing such variants.

### 5 BACKGROUND OF THE INVENTION

Maltogenic alpha-amylase (glucan 1,4- $\alpha$ -maltohydrolase, E.C. 3.2.1.133) is able to hydrolyze amylose and amylopectin to maltose in the alpha-configuration, and is also able to hydrolyze maltotriose as well as cyclodextrin.

10 A maltogenic alpha-amylase from *Bacillus* (EP 120 693) is commercially available under the trade name Novamyl® (product of Novo Nordisk A/S, Denmark) and is widely used in the baking industry as an anti-staling agent due to its ability to reduce retrogradation of starch (WO 91/04669). It is most active at 60-70°C (Christophersen, C., et al., 1997, Starch, vol. 50, No. 1, 39-45).

Novamyl® shares several characteristics with cyclodextrin glucanotransferases 15 (CGTases), including sequence homology (Henrissat B., Bairoch A. 1996) and formation of transglycosylation products (Christophersen, C., et al., 1997, Starch, vol. 50, No. 1, 39-45). Cyclomaltodextrin glucanotransferase (E.C. 2.4.1.19), also designated cyclodextrin glucanotransferase or cyclodextrin glycosyltransferase, abbreviated herein as CGTase, catalyses the conversion of starch and similar 20 substrates into cyclomaltodextrins via an intramolecular transglycosylation reaction, thereby forming cyclomaltodextrins (or CD) of various sizes.

CGTases are widely distributed and from several different bacterial sources, including *Bacillus*, *Brevibacterium*, *Clostridium*, *Corynebacterium*, *Klebsiella*, *Micrococcus*, *Thermoanaerobacter* and *Thermoanaerobacterium* have been 25 extensively described in the literature. A CGTase produced by *Thermoanaerobacter* sp. has been reported in Norman B E, Jørgensen S T; Denpun Kagaku 1992 39 99-106, and WO 89/03421, and the amino acid sequence has been disclosed in WO 96/33267. The sequence of CGTases from *Thermoanaerobacterium thermosulfurigenes* and from *Bacillus circulans* available on the Internet (SCOP or PDF home pages) as pdf file 30 1CIU, and the sequence of a CGTase from *B. circulans* is available as pdf file 1CDG.

Tachibana, Y., Journal of Fermentation and Bioengineering, 83 (6), 540-548 (1997) describes the cloning and expression of a CGTase. Variants of CGTases have been described by Kim, Y. H., Biochemistry and Molecular Biology International, 41 (2), 227-234 (1997); Sin K-A, Journal of Biotechnology, 32 (3), 283-288 (1994); D 35 Penninga, Biochemistry, 34 (10), 3368-3376 (1995); and WO 96/33267.

Recently, the tertiary structure of several CGTases have been reported. Hofman et al. [Hofman B E, Bender H, Schultz G E; J. Mol. Biol. 1989 209 793-800] and Klein &

Schulz [Klein C, Schulz G E; J. Mol. Biol. 1991 **217** 737-750] report the tertiary structure of a CGTase derived from *Bacillus circulans* Strain 8, Kubota et al. [Kubota M, Matsuura Y, Sakai S and Katsube Y; Denpun Kagaku 1991 **38** 141-146] report the tertiary structure of a CGTase derived from *Bacillus stearothermophilus* TC-91, Lawson et al. [Lawson C L, van Montfort R, Strokopytov B, Rozeboom H J, Kalk K H, de Vries G E, Penninga D, Dijkhuizen L, and Dijkstra B W; J. Mol. Biol. 1994 **236** 590-600] report the tertiary structure of a CGTase derived from *Bacillus circulans* Strain 251, Strokopytov et al. [Strokopytov B, Penninga D, Rozeboom H J; Kalk K H, Dijkhuizen L and Dijkstra B W; Biochemistry 1995 **34** 2234-2240] report the tertiary structure of a CGTase derived from *Bacillus circulans* Strain 251, which CGTase has been complexed with acarbose, an effective CGTase inhibitor, and Knegt et al. [Knegtel R M A, Wind R D, Rozeboom H J, Kalk K H, Buitelaar R M, Dijkhuizen L and Dijkstra B W; J. Mol. Biol. 1996 **256** 611-622] report the tertiary structure of a CGTase derived from *Thermoanaerobacterium thermosulfurigenes*.

## 15 BRIEF DISCLOSURE OF THE INVENTION

The inventors have found that the anti-staling effect of a maltogenic amylase can be improved by using a variant having increased thermostability. Further, they found that such a variant improves the softness of baked products in the initial period after baking, particularly the first 24 hours after baking, so that the baked product has improved softness, both when eaten on the same day and when stored for several days after baking.

Accordingly, the invention provides a polypeptide which:

- a) has maltogenic amylase activity;
- b) has at least 70 % identity to SEQ ID NO: 1,
- 25 c) has optimum maltogenic amylase activity in the range pH 3.5-7.0 (preferably 4-5.5), and
- d) shows a residual maltogenic amylase activity of at least 25 % after incubation with 1 mM Ca<sup>++</sup> at pH 4.3, 80°C for 15 minutes.

The inventors found that thermostable variants can be prepared by random DNA mutagenesis followed by screening for thermostable variants. Thus, the invention also provides a method of preparing a maltogenic amylase variant having improved anti-staling properties, which method comprises

- a) subjecting a DNA sequence encoding the maltogenic amylase to random mutagenesis,
- 35 b) expressing the mutated DNA sequence obtained in step (a) in a host cell, and
- c) screening for host cells expressing a mutated maltogenic amylase which shows a higher thermostability, and

d) preparing the mutated maltogenic amylase expressed by the host cells.

Further, the inventors have modified the amino acid sequence of a maltogenic alpha-amylase to obtain variants with improved properties, based on the three-dimensional structure of the maltogenic alpha-amylase Novamyl. The variants have altered physicochemical properties., e.g. an altered pH optimum, improved thermostability, increased specific activity, an altered cleavage pattern or an increased ability to reduce retrogradation of starch or staling of bread.

Accordingly, the present invention provides a method of constructing a variant of a parent maltogenic alpha-amylase, wherein the variant has at least one altered property as compared to said parent maltogenic alpha-amylase, which method comprises:

i) analyzing the structure of the maltogenic alpha-amylase to identify, on the basis of an evaluation of structural considerations, at least one amino acid residue or at least one structural region of the maltogenic alpha-amylase, which is of relevance for altering said property;

ii) constructing a variant of the maltogenic alpha-amylase, which as compared to the parent, has been modified in the amino acid residue or structural part identified in i) so as to alter said property; and

iii) testing the resulting maltogenic alpha-amylase variant for said property.

The property which may be altered by the above methods of the present invention may be, e.g., stability, pH dependent activity, ability to reduce retrogradation of starch or staling of bread, specific activity, or substrate specificity. Thus, the variant may have, e.g., increased thermostability or higher activity at a lower pH an altered pH optimum, improved thermostability, increased specific activity or increased ability to reduce retrogradation of starch or staling of bread

In still further aspects the invention relates to variants of a maltogenic alpha-amylase, the DNA encoding such variants and methods of preparing the variants. Finally, the invention relates to the use of the variants for various industrial purposes, in particular baking.

## DETAILED DISCLOSURE OF THE INVENTION

### Maltogenic alpha-amylase

The maltogenic alpha-amylase is an enzyme classified in EC 3.2.1.133. The enzymatic activity does not require a non-reducing end on the substrate and the primary enzymatic activity results in the degradation of amylopectin and amylose to maltose and longer maltodextrins. It is able to hydrolyze amylose and amylopectin to maltose in the alpha-configuration, and is also able to hydrolyze maltotriose as well as cyclodextrin.

A particularly preferred maltogenic alpha-amylase is the amylase cloned from *Bacillus* as described in EP 120 693 (hereinafter referred to as Novamyl). Novamyl has the amino acid sequence set forth in amino acids 1-686 of SEQ ID NO: 1. Novamyl is encoded in the gene harbored in the *Bacillus* strain NCIB 11837 which has the nucleic acid sequence set forth in SEQ ID NO:1. The three-dimensional structure of Novamyl is described below.

In general, a preferred maltogenic alpha-amylase should have one or more of the following properties:

- i) a three dimensional structural homology to Novamyl,
- 10 ii) an amino acid sequence having at least 70 % identity to SEQ ID NO: 1, preferably at least 80 % or 90 %, e.g. 95 % or 98 %,
- iii) a DNA sequence which hybridizes to the DNA sequence set forth in SEQ ID NO:1 or to the DNA sequence encoding Novamyl harbored in the *Bacillus* strain NCIB 11837;
- 15 iv) a calcium binding site comprising a coordination equivalent to a backbone carbonyl atom from Asn77, sidechain atom OE2 and OE1 from Glu102, a sidechain atom OD1 from Asp79, a sidechain atom OD1 from Asp76, and a sidechain atom OE1 from Glu101, and one water molecule WAT V21, atom OW0, wherein the positions are as shown in Appendix 1;
- 20 v) a sequence of five amino acids corresponding to Pro-Ala-Gly-Phe-Ser in a position equivalent to residues 191-195 in the amino acid sequence shown in SEQ ID NO: 1; and

The structural homology referred to above in i) is based on other sequence homologies, hydrophobic cluster analysis or by reverse threading (Huber, T ; Torda, 25 AE, PROTEIN SCIENCE Vol. 7 , No. 1 pp. 142-149 (1998)) and which by any of these methods is predicted to have the same tertiary structure as Novamyl, wherein the tertiary structure refers to the overall folding or the folding of Domains A, B, and C, more preferably including Domain D, and most preferably including Domain E. Alternatively, a structural alignment between Novamyl and a maltogenic alpha-amylase 30 may be used to identify equivalent positions.

The calcium binding site referred to above in iv) is based on a calcium binding site identified in the three-dimensional structure of Novamyl, and is discussed below in the section "Calcium binding sites."

The "equivalent position" referred to above in v) is based on amino acid or DNA 35 sequence alignment or structural homology using methods known in the art.

### Three-dimensional structure of maltogenic alpha-amylase

Novamyl was used to elucidate the three-dimensional structure forming the basis for the present invention.

The structure of Novamyl was solved in accordance with the principle for x-ray crystallographic methods, for example, as given in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989.

The structural coordinates for the solved crystal structure of Novamyl at 2.2 Å resolution using the isomorphous replacement method are given in standard PDB format (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT) as set forth in Appendix 1. It is to be understood that Appendix 1 forms part of the present application. In the context of Appendix 1, the following abbreviations are used: CA refers to calcium ion or alpha-carbon atom of the polypeptide backbone, WAT refers to water or to calcium, MAL refers to maltose, HEX refers to a carbohydrate unit of a substrate analogue, and SUL refers to a sulfate ion.

Amino acid residues of the enzyme are identified herein by their respective one- or three-letter amino acid code.

The structure of said maltogenic alpha-amylase is made up of five globular domains, ordered A, B, C, D and E. The domains can be defined as being residues 1-132 and 204-403 for Domain A, residues 133-203 for Domain B, residues 404-496 for Domain C, residues 497-579 for Domain D, and residues 580-686 for Domain E, wherein the numbering refers to the amino acid sequence in SEQ ID NO: 1. Features of Domains A, B, and C of particular interest are described below.

## 20 Domain A

Domain A is the largest domain and contains the active site which comprises a cluster of three amino acid residues, D329, D228 and E256, spatially arranged at the bottom of a cleft in the surface of the enzyme. The structure of Domain A shows an overall fold in common with the  $\alpha$ -amylases for which the structure is known, viz. the (beta/alpha) 8 barrel with eight central beta strands (numbered 1-8) and eight flanking a-helices. The  $\beta$ -barrel is defined by McGregor *op. cit.* The C-terminal end of the beta strand 1 is connected to helix 1 by a loop denoted loop 1 and an identical pattern is found for the other loops, although the loops show some variation in size and some can be quite extensive.

30 The eight central beta-strands in the (beta/alpha) 8 barrel superimpose reasonably well with the known structures of CGTases. This part of the structure, including the close surroundings of the active site located at the C-terminal end of the beta-strands, shows a high degree of identity with CGTases.

In contrast, the loops connecting the beta-strands and alpha helices display a high degree of variation from the known structures of CGTases. These loops constitute the structural context of the active site, and the majority of the contacts to the substrate is found among residues located in these loops. Distinguishing characteristics such as substrate specificity, substrate binding, pH activity profile, substrate cleavage pattern,

and the like, are determined by specific amino acids and the positions they occupy in these loops. In Novamyl Domain A contains two calcium binding sites, one of which is homologous to the calcium binding site in CGTases; the other is unique to Novamyl. The structure of the calcium binding site is discussed further below in the section

## 5 "Calcium binding sites."

### Domain B

Domain B, also referred to as loop 3 of the (beta/alpha) 8 barrel, in comprises amino acid residues 133-203 of the amino acid sequence shown in SEQ ID NO: 1. The structure is partially homologous to the structure of Domain B in CGTases, the most striking difference being the presence of a five amino acid insert corresponding to positions 191-195 in the amino acid sequence shown in SEQ ID NO: 1 which is not found in the CGTases. This insert is spatially positioned close to the active site residues and in close contact to the substrate.

### Domain C

15 Domain C in Novamyl comprises amino acid residues 404-496 of the amino acid sequence shown in SEQ ID NO: 1. Domain C is composed entirely of  $\beta$ -strands which form a single 8-stranded sheet structure that folds back on itself, and thus may be described as a  $\beta$ -sandwich structure. One part of the  $\beta$ -sheet forms the interface to Domain A.

## 20 Calcium binding sites

The structure of the maltogenic alpha-amylase exhibits three calcium-binding sites; that is, three calcium ions are found to be present in the structure. In common with most of the known family 13 structures, one calcium ion, WAT 693 in Appendix 1, is located between the A and B domains. This calcium ion is coordinated by a backbone carbonyl atom from Gln184 and His232, sidechain atoms OD2 and OD1 from Asp198, a sidechain atom OD1 from Asn131, and three water molecules WAT V1, WAT V5 and WAT V8.

A second calcium ion is located in the A domain and is common to CGTases, but not found in  $\alpha$ -amylases. The calcium ion WAT 694 is coordinated by a backbone carbonyl atom from Gly48 and Asp23, sidechain atom OD2 from Asp50, a sidechain atom OD1 from Asp21, a sidechain atom OD1 from Asn26, and a sidechain atom OD1 from Asn27, and one water molecule WAT V62.

The third calcium ion is located in the A Domain and is unique to Novamyl. The calcium ion is WAT 692 and the coordination comprises a backbone carbonyl atom from Asn77, sidechain atom OE2 and OE1 from Glu102, a sidechain atom OD1 from

Asp79, a sidechain atom OD1 from Asp76, and a sidechain atom OE1 from Glu101, and one water molecule WAT V21.

### Substrate Binding Site

Parts of the loop discussed above in the context of domains A and B are of particular interest for substrate interaction and active site reactivity. In particular, in domain A, residues 37-45 in loop 1, residues 261-266 in loop 5, residues 327-330 in loop 7 and residues 370-376 in loop 8; in domain B, residues 135-145 in loop 3, residues 173-180 and 188-196 in loop 3, wherein residue positions correspond to the amino acids in the amino acid sequence in SEQ ID NO: 1.

Without being limited to any theory, it is presently believed that binding between a substrate and an enzyme is supported by favorable interactions found within a sphere of 4 to 6 Å between the substrate molecule and the enzyme, such as hydrogen bonds and/or strong electrostatic interaction. The following residues of Novamyl (SEQ ID NO: 1), are within a distance of 6 Å of the substrate HEX and thus believed to be involved in interactions with said substrate:

44, 89, 90, 92, 93, 127, 129, 132, 135, 177, 178, 188, 191, 194, 196, 226, 228, 229, 230, 231, 232, 256, 258-261, 288, 328, 329, 371, 372, 373, 376, and 690.

The following residues of Novamyl are within a distance of 4 Å of the substrate HEX and thus believed to be involved in interactions with said substrate:

90, 92, 93, 129, 132, 177, 188, 189, 190, 191, 196, 226, 228, 229, 231, 232, 256, 258, 259, 260, 261, 328, 329, 372, 376, and 690.

### **Homology building of Novamyl®**

The structure of the Novamyl® was model built on the structure disclosed in Appendix 1 herein. The structure of other maltogenic alpha-amylases may be built analogously.

A model structure of a maltogenic alpha-amylase can be built using the Homology program or a comparable program, eg., Modeller (both from Molecular Simulations, Inc., San Diego, CA). The principle is to align the sequence of the maltogenic alpha-amylase with the known structure with that of the maltogenic alpha-amylase for which a model structure is to be constructed. The structurally conserved regions can then be built on the basis of consensus sequences. In areas lacking homology, loop structures can be inserted, or sequences can be deleted with subsequent bonding of the necessary residues using, e.g., the program Homology. Subsequent relaxing and optimization of the structure should be done using either Homology or another molecular simulation program, e.g., CHARMM from Molecular Simulations.



## Methods for designing novel maltogenic alpha-amylase variants

In a first aspect, the invention relates to a method of constructing a variant of a parent maltogenic alpha-amylase, wherein said variant has at least one altered property as compared to said parent  $\alpha$ -amylase, which method comprises:

- 5 i) analyzing the structure of the maltogenic alpha-amylase to identify at least one amino acid or structural region of said  $\alpha$ -amylase, which, on the basis of structural or functional considerations, is determined to be of relevance for altering said property of the parent maltogenic alpha-amylase;
- ii) constructing a variant of the maltogenic alpha-amylase, which as compared  
10 to the parent, has been modified in the amino acid residue or structural region identified in i) has been modified so as to alter said property; and
- iii) testing the resulting variant for said property.

The structural part which is identified in step i) of the method of the invention may be composed of one amino acid residue. However, normally the structural part  
15 comprises more than one amino acid residue, typically constituting one of the above parts of the maltogenic alpha-amylase structure such as one of the A, B, C, D or E domains, an interface between any of these domains, a calcium binding site, a loop structure, the substrate binding site, or the like.

The structural or functional considerations may involve an analysis of the  
20 relevant structure or structural part and its contemplated impact on the function of the enzyme. For example, an analysis of the functional differences between maltogenic alpha-amylase and the various CGTases may be used for assigning certain properties of Novamyl to certain parts of the Novamyl structure or to contemplate such relationship. For instance, differences in the pattern or structure of loops surrounding  
25 the active site may result in differences in access to the active site of the substrate and thus differences in substrate specificity and/or cleavage pattern.

Furthermore, parts of a maltogenic alpha-amylase involved in substrate binding, and thus, for example, substrate specificity and/or cleavage, calcium ion binding, important, for example, for the calcium dependency of the enzyme, and the  
30 like, have been identified (*vide infra*).

The modification of an amino acid residue or structural region is typically accomplished by suitable modifications of a DNA sequence encoding the parent enzyme in question. The modification may be substitution, deletion or insertion of an amino acid residue or a structural part.

35 The property to be modified may be stability (e.g. thermostability), pH dependent activity, substrate specificity, specific activity or ability to reduce retrogradation of starch or staling of bread. Thus, the altered property may be an altered specific activity at a given pH and/or an altered substrate specificity, such as an altered pattern of substrate cleavage or an altered pattern of substrate inhibition.

In step ii) of the method according to the invention the part of the structure to be identified is preferably one which in the folded enzyme is believed to be in contact with the substrate (cf, the disclosure above in the section entitled "Substrate Binding Site") or involved in substrate specificity and/or cleavage pattern, and/or one which is in contact with one of the calcium ions and/or one, which is contributing to the pH or temperature profile of the enzyme, or is otherwise responsible for the properties of the maltogenic alpha-amylase.

Described in the following are specific types of variants which have been designed by use of the method of the invention.

The variants of the invention may comprise additional modifications in addition to the modifications described herein. The variants preferably have an amino acid having more than 70 % identity with SEQ ID NO: 1, preferably more than 80 %, particularly more than 90 %, especially more than 95 %, e.g. more than 98 %.

#### **Maltogenic alpha-amylase variants with altered pH dependent activity profile**

The pH dependent activity profile can be changed by changing the pKa of residues within 10 Å of the active site residues of the maltogenic alpha-amylase. Changing the pKa of the active site residues is achieved, e.g., by changing the electrostatic interaction or hydrophobic interaction between functional groups of amino acid side chains of a given amino acid residue and its close surroundings. To obtain a higher activity at a higher pH, negatively charged residues are placed near a hydrogen donor acid, whereas positively charged residues placed near a nucleophilic acid will result in higher activity at low pH. Also, a decrease in the pKa can be obtained by reducing the accessibility of water or increasing hydrophobicity of the environment.

Thus, another aspect of the present invention relates to a variant of a parent maltogenic alpha-amylase, in which the variant has an altered pH dependent activity profile as compared to the parent, wherein the variant may be obtained by the following method:

i) identifying an amino acid residue within 15 Å from an active site residue of a maltogenic alpha-amylase in the three-dimensional structure of said parent maltogenic alpha-amylase, in particular 10 Å from an active site residue, wherein said amino acid residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site residue;

ii) substituting, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue, and evaluating the accommodation of the amino acid residue in the structure,

iii) optionally repeating step i) and/or ii) recursively until an amino acid substitution has been identified which is accommodated into the structure,

iv) constructing a maltogenic alpha-amylase variant resulting from steps i) and ii), and optionally iii), and testing the pH dependent enzymatic activity of said variant.

In a preferred embodiment, the variant of a maltogenic alpha-amylase having an altered pH dependent activity profile as compared to the parent maltogenic alpha-amylase comprises a modification of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

D127, V129, F188, A229, Y258, V281, F284, T288, N327, M330, G370, N371, and D372,

L71, S72, V74, L75, L78, T80, L81, G83, T84, D85, N86, T87, G88, Y89, H90, G91, T94, R95, D96, F97, I174, S175, N176, D178, D179, R180, Y181, E182, A183, Q184, K186, N187, F188, T189, D190, A192, G193, F194, S195, L196.

In more preferred embodiment, the variant comprises a modification corresponding to one or more of the following modifications in the amino acid sequence set forth in SEQ ID NO: 1:

D127N/L, V129S/T/G/V, F188E/K/H, A229S/T/G/V, Y258E/D/K/R/F/N, V281L/T, F284K/H/D/E/Y, T288E/K/R, N327D, M330L/F/I/D/E/K, G370N, N371D/E/G/K, and D372N/V,

L71I, S72C, V74I, L75N/D/Q/I/V, L78N/I, T80I/L/V/S/N/G, L81I/V/S/T/N/Q/K/H, G83A/S/T/N/Q/E/D/R/H/L, T84S/A/N/D/G, D85A/T/S/N/G, N86Q/E/D/Y/H/K, T87S/I, G88A/S/T, Y89F, H90N/Q/K, G91A/S/T, T94N/D/A/M/V/I, R95K/Q, D96N/V/Q/I, F97Y, I174N/Q/L, S175T/A/N/D, N176S/T/H/Q/P, D178N/Q/E/K/H, D179Y/N/H, R180W, Y181R/F/C/L, E182D, A183S/C/G, Q184E, K186R, N187Q/E/L/F/H/K/V/L, F188Y/L/I/H/N, T189N/D/A/S/H/Y/G, D190E/Q/H/N/K, A192T/D/E/N/K, G193A/S/T, F194Y, S195N/D/E/R/K/G, L196I.

Similar modifications may be introduced in equivalent positions of other maltogenic alpha-amylases. Variants of particular interest have a combination of one or more of the above with any of the other modifications disclosed herein.

### **Maltogenic alpha-amylase variants with altered stability**

A variant with improved stability (typically increased stability) may be obtained by stabilization of calcium binding, substitution with proline, substitution of histidine with another amino acid, introduction of an interdomain disulfide bond, removal of a deamidation site, altering a hydrogen bond contact, filling in an internal structural cavity with one or more amino acids with bulkier side groups, introduction of interdomain interactions, altering charge distribution, helix capping, or introduction of a salt bridge.

### **Calcium binding**

The invention provides a variant of a parent maltogenic alpha-amylase, which has an altered stability due to an altered stabilization of calcium ( $\text{Ca}^{2+}$ ) binding. The

enzyme variant may have altered thermostability or pH dependent stability, or it may have maltogenic alpha-amylase activity in the presence of a lower concentration of calcium ion. It is presently believed that amino acid residues located within 10 Å from a calcium ion are involved in or are of importance for the Ca<sup>2+</sup> binding capability of the enzyme.

The amino acid residues found within a distance of 10 Å from the Ca<sup>2+</sup> binding sites of the maltogenic alpha-amylase with the amino acid sequence set forth in SEQ ID NO: 1 were determined as described in Example 2 and are as follows:

16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 35, 36, 40, 46, 47, 48, 49, 50, 51, 52, 53, 54, 56, 73, 74, 75, 76, 77, 78, 79, 80, 81, 87, 88, 89, 91, 93, 94, 95, 96, 99, 100, 101, 102, 103, 104, 105, 109, 129, 130, 131, 132, 133, 134, 145, 150, 167, 168, 169, 170, 171, 172, 174, 177, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 196, 197, 198, 199, 200, 201, 202, 206, 210, 228, 229, 230, 231, 232, 233, 234, 235, 237, 378, and 637.

In order to construct a variant according to this aspect of the invention it is desirable to substitute at least one of the above mentioned amino acid residues, which is determined to be involved in a non-optimal calcium binding, with any other amino acid residue which improves the Ca<sup>2+</sup> binding affinity of the variant enzyme. Accordingly, another aspect of the invention relates to a method of constructing a variant of a parent maltogenic alpha-amylase wherein said variant has a stabilised Ca<sup>2+</sup> binding as compared to said parent, which method comprises:

i) identifying an amino acid residue within 10 Å from a Ca<sup>2+</sup> binding site of a maltogenic alpha-amylase in a model of the three-dimensional structure of said α-amylase which, from structural or functional considerations, is determined to be responsible for a non-optimal calcium ion interaction;

ii) constructing a variant in which said amino acid residue is substituted with another amino acid residue which, from structural or functional considerations, is determined to be important for establishing an altered Ca<sup>2+</sup> binding affinity; and

iii) testing the Ca<sup>2+</sup> binding of the resulting maltogenic alpha-amylase variant.

Substituting an amino acid residue responsible for non-optimal calcium ion interaction with another residue may alter a calcium ion binding interaction of the enzyme. For instance, the amino acid residue in question may be selected on the basis of one or more of the following objectives:

a) to obtain an improved interaction between a calcium ion and an amino acid residue as identified from the structure of the maltogenic alpha-amylase. For instance, if the amino acid residue in question is exposed to a surrounding solvent, it may be advantageous to increase the shielding of said amino acid residue from the solvent so as to stabilize the interaction between said amino acid residue and a calcium ion. This can be achieved by substituting said residue, or an amino acid residue in the vicinity of

said residue contributing to the shielding, with an amino acid residue with a bulkier side group or which otherwise results in an improved shielding effect.

b) to stabilize a calcium binding site, for instance by stabilizing the structure of the maltogenic alpha-amylase, e.g. by stabilizing the contacts between two or more of the five domains or stabilizing one or more of the individual domains as such. This may, e.g., be achieved by providing for a better coordination to amino acid side chains, which may, e.g., be obtained by substituting an N residue with a D residue and/or a Q residue with an E residue, e.g. within 10 Å, and preferably within 3 or 4 Å, of a calcium binding site.

c) to improve the coordination between the calcium ion and the calcium binding residues, e.g., by improving the interaction between the ion and the coordinating residues or increasing the number of sidechain coordinations by substituting a coordinating water with an amino acid sidechain.

d) replace water by a coordinating calcium amino acid residue.

Preferably, the amino acid residue to be modified is located within 8 Å of a  $\text{Ca}^{2+}$  ion, preferably within 5 Å of a  $\text{Ca}^{2+}$  ion. The amino acid residues within 8 Å and 5 Å, respectively, may easily be identified by an analogous method used for identifying amino acid residues within 10 Å (cf. Example 2).

In a preferred embodiment, the variant of a maltogenic alpha-amylase having an altered  $\text{Ca}^{2+}$  binding as compared to the parent maltogenic alpha-amylase comprises a substitution of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

D17, A30, S32, R95, H103, N131, Q201, I174, and/or H169,

V74, L75, L78, T80, L81, T87, G88, Y89, H90, G91, T94, R95, D96, F97, Y167, F168, H169, H170, N171, G172, D173, I174, S175, N176, D178, D179, R180, Y181, E182, A183, Q184, K186, N187, F188, T189.

In more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to one or more of the following substitutions in the amino acid sequence set forth in SEQ ID NO: 1:

D17E/Q, A30M/L/A/V/I/E/Q, S32D/E/N/Q, R95M/L/A/V/I/E/Q, H103Y/N/Q/D/E, N131D, Q201E, I174E/Q, and H169N/D/E/Q

V74I, L75N/D/Q/I/V, L78N/I, T80I/L/V/S/N/G, L81I/V/S/T/N/Q/K/H, T87S/I, G88A/S/T, Y89F, H90N/Q/K, G91A/S/T, T94N/D/A/M/V/I, R95K/Q, D96N/V/Q/I, F97Y, Y167F/R/C, F168Y, H169N/Q/K, H170N/Q/K, N171D/E/Q/H/R/K/G, G172A/T/S, D173N/S/T/Y/R/G, I174N/Q/L, S175T/A/N/D, N176S/T/H/Q/P, D178N/Q/E/K/H, D179Y/N/H, R180W, Y181R/F/C/L, E182D, A183S/C/G, Q184E, K186R, N187Q/E/L/F/H/K/V/L, F188Y/L/I/H/N, T189N/D/A/S/H/Y/G.

In another preferred embodiment of the invention with respect to altering the  $\text{Ca}^{2+}$  binding of a maltogenic alpha-amylase the partial sequence N28-P29-A30-K31-S32-Y33-G34 as set forth in SEQ ID NO: 1 is modified.

Similar substitutions may be introduced in equivalent positions of other maltogenic alpha-amylases. Modifications of particular interest are any combination of one or more of the above with any of the other modifications disclosed herein.

#### Other substitutions

Variants with improved stability of the enzyme can be achieved by improving existing or introducing new interdomain and intradomain contacts. Such improved stability can be achieved by the modifications listed below.

The maltogenic alpha-amylase having the amino acid sequence shown in SEQ ID NO: 1 may be stabilized by the introduction of one or more interdomain disulfide bonds. Accordingly, another preferred embodiment of the present invention relates to a variant of a parent maltogenic alpha-amylase which has improved stability and at least one more interdomain disulfide bridge as compared to said parent, wherein said variant comprises a modification in a position corresponding to at least one of the following pairs of positions in SEQ ID NO: 1:

G236 + S583, G618 + R272, T252 + V433 and/or A348 + V487.

In a more preferred embodiment, the substitution corresponds to at least one of the following pairs:

G236C + S583C, G618C + R272C, T252C + V433C and/or A348C + V487C.

Another preferred embodiment of the invention relates to a variant of a parent maltogenic alpha-amylase which has an improved stability and an altered interdomain interaction as compared to said parent, wherein said variant comprises a substitution in a position corresponding at least one of the following sets of positions in SEQ ID NO: 1:

i) F143, F194, L78;

ii) A341, A348, L398, I415, T439, L464, L465;

iii) L557;

iv) S240, L268;

v) Q208, L628;

vi) F427, Q500, N507, M508, S573; and

vii) I510, V620.

In a more preferred embodiment, the substitution corresponds to at least one of the following sets:

i) F143Y, F194Y, L78Y/F/W/E/Q;

ii) A341S/D/N, A348V/I/L, L398E/Q/N/D, I415E/Q, T439D/E/Q/N, L464D/E, L465D/E/N/Q/R/K;

iii) L557Q/E/N/D;

iv) S240D/E/N/Q, L268D/E/N/Q/R/K;

v) Q208D/E/Q, L628E/Q/N/D;

vi) F427E/Q/R/K/Y, Q500Y, N507Q/E/D, M508K/R/E/Q, S573D/E/N/Q; and/or

vii) I510D/E/N/Q/S, V620D/E/N/Q.

5 Another preferred embodiment of the invention relates to a variant of a parent maltogenic alpha-amylase which has an improved stability and one or more salt bridges as compared to said parent, wherein said variant comprises a substitution in a position corresponding at least one of the following sets of positions in SEQ ID NO: 1:

N106, N320 and Q624.

10 In a more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to the following substitutions in the amino acid sequence set forth in SEQ ID NO: 1:

N106R, N320E/D and/or Q624E.

Another embodiment of the invention relates to a variant of a parent maltogenic  
15 alpha-amylase which has an improved stability and wherein said variant comprises a substitution in a position corresponding at least one of the following sets of positions in SEQ ID NO: 1:

K40, V74, S141, T142, F188, N234, K249, D261, D261, L268, V279, N342,  
G397, A403, K425, S442, S479, S493, T494, S495, A496, S497, A498, Q500, K520,  
20 A555 and N595.

In a more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to one or more of the following substitutions with proline in the amino acid sequence set forth in SEQ ID NO: 1:

V74P, S141P, N234P, K249P, L268P, V279P, N342P, G397P, A403P, S442P,  
25 S479P, S493P, T494P, S495P, A496P, S497P, A498P, Q500P, and/or A555P.

Other preferred substitutions are K40R, T142A, F188I/L, D261G, K425E, K520R, and/or N595I.

Analogously, it may be preferred that one or more histidine residues present in the parent maltogenic alpha-amylase is or are substituted with a non-histidine residues  
30 such as Y, V I, L, F, M, E, Q, N, or D. Accordingly, in another preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

H103, H220, and H344

35 In a more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to one or more of the following substitutions in the amino acid sequence set forth in SEQ ID NO: 1:

H103Y/V/I/L/F/Y, H220Y/L/M, and H344E/Q/N/D/Y.

It may be preferred that one or more asparagine or glutamine residues present in the parent maltogenic alpha-amylase is or are substituted with a residue lacking the amide on the side chain. Accordingly, in another preferred embodiment, the variant of a Novamyl-like comprises a substitution of an amino acid residue corresponding to one or  
5 more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

Q13, N26, N77, N86, N99, Q119, N120, N131, N152, N171, N176, N187, Q201, N203, N234, Q247, N266, N275, N276, N280, N287, Q299, N320, N327, N342, Q365, N371, N375, N401, N436, N454, N468, N474, Q500, N507, N513, Q526, N575, Q581, N621, Q624 and N664.

10 In more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to one or more of the following substitutions in the amino acid sequence set forth in SEQ ID NO: 1:

Q13S/T/A/V/L/I/F/M, N26S/T/A/V/L/I, N77S/T/A/V/L/I, N86S/T/A/V/L/I, N99T/S/V/L, Q119T/S, N120S/T/A/V/L/I, N131S/T/A/V/L/I, N152T/S/V/L, N171Y/D/S/T,  
15 N176S/T/A/V/L/I, N187S/T/A/V/L/I, Q201S/T/A/V/L/I/F/M, N203D/S/T/A/V/L/I, N234S/T/A/V/L/I, Q247S/T/A/V/L/I/F/M, N266S/T/A/V/L/I, N275S/T/A/V/L/I, N276S/T/A/V/L/I, N280S/T/A/V/L/I, N287S/T/A/V/L/I, Q299L/T/S, N320S/T/A/V/L/I, N327S/T/A/V/L/I, N342S/T/A/V/L/I, Q365S/T/A/V/L/I, N371S/T/A/V/L/I, N375S/T/A/V/L/I, N401S/T/A/V/L/I, N436S/T/A/V/L/I, N454D/S/T/A/V/L/I, N468D/S/T/A/V/L/I,  
20 N474D/S/T/A/V/L/I, Q500S/T/A/V/L/I/F/M, N507S/T/A/V/L/I, N513S/T/A/V/L/I, Q526D/S/T/A/V/L/I, N575S/T/A/V/L/I, Q581S/T/A/V/L/I/F/M, N621S/T/A/V/L/I, Q624S/T/A/V/L/I/F/M and N664D/S/T/A/V/L/I.

Another embodiment of the invention relates to a variant of a parent maltogenic alpha-amylase which has improved stability and improved hydrogen bond contacts as  
25 compared to said parent, wherein said variant comprises a modification in a position corresponding to one or more of the following positions in SEQ ID NO: 1:

I16, L35, M45, P73, D76, D79, A192, I100, A148, A163+G172, L268, V281, D285, L321, F297, N305, K316, S573, A341, M378, A381, F389, A483, A486, I510, A564, F586, K589, F636, K645, A629, and/or T681.

30 In a preferred embodiment, the modification corresponds to one or more of the following:

I16T/D/N, L35Q, M45K, P73Q, D76E, D79E/Y, A192S/D/N, I100T/S/D/N/E/Q, A148D/N/E/Q/S/T/R/K, A163Y+G172S/D/N, L268R/K, V281/Q, D285R/K, L321Q, F297N/D/Q/E, N305K/R, K316N/D, S573N/D, A341R/K, M378R/K, A381S/D/N, F389Y,  
35 A483S/D/N, A486Q/E, I510R/K, A564S/D/N, F586S/D/N, K589S/D/Q/N, F636Y, K645T, A629N/D/E/Q, and/or T681D/N/E/Q/S.

Similar substitutions may be introduced in equivalent positions of other maltogenic alpha-amylases. Substitutions of particular interest are any combination of one or more of the above with any of the other modifications disclosed herein.



Before actually constructing a maltogenic alpha-amylase variant to achieve any of the above objectives, it may be convenient to evaluate whether or not the contemplated amino acid modification can be accommodated into the maltogenic alpha-amylase structure, e.g. into a model of the three-dimensional structure of the parent maltogenic alpha-amylase.

### **Maltogenic alpha-amylase variants with altered thermostability and/or altered temperature dependent activity profile**

The invention further relates to a variant of a parent maltogenic alpha-amylase, which results from substitution, deletion or insertion of one or more amino acid residues so as to obtain a variant having an altered thermostability or temperature dependent activity profile.

The structure of the maltogenic alpha-amylase contains a number of unique internal cavities which may contain water and a number of crevices. In order to increase the thermostability of the polypeptide it may be desirable to reduce the number or size of cavities and crevices, e.g., by introducing one or more hydrophobic contacts, preferably achieved by introducing amino acids with bulkier side groups in the vicinity or surroundings of the cavity. For instance, the amino acid residues to be modified are those which are involved in the formation of the cavity.

Accordingly, in a further aspect the present invention relates to a method of increasing the thermostability and/or altering the temperature dependent activity profile of a parent maltogenic alpha-amylase, which method comprises:

- i) identifying an internal cavity or a crevice of the parent maltogenic alpha-amylase in the three-dimensional structure of said polypeptide;
- ii) substituting, in the structure, one or more amino acid residues in the neighbourhood of the cavity or crevice identified in step i) with another amino acid residue which, from structural or functional considerations, is determined to increase the hydrophobic interaction and to fill out or reduce the size of the cavity or crevice; and
- iii) constructing a variant of the parent maltogenic alpha-amylase resulting from step ii) and testing the thermostability and/or temperature dependent activity of the variant.

The structure identified in Appendix 1 may be used for identifying the cavity or crevice of the parent maltogenic alpha-amylase.

It will be understood that the cavity or crevice is identified by the amino acid residues surrounding said cavity or crevice, and that modification of said amino acid residues are of importance for filling or reducing the size of said cavity or crevice. Preferably, the modification is a substitution with a bulkier amino acid residue, i.e. one with a greater side chain volume. For example, all the amino acids are bulkier than Gly, whereas Tyr and Trp are bulkier than Phe. The particular amino acid residues referred

to below are those which in a crystal structure have been found to flank the cavity or crevice in question.

In a preferred embodiment, the variant of a maltogenic alpha-amylase, in order to fill, either completely or partly, cavities located internally in the structure, comprises a  
5 substitution of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

L51, L75, L78, G88, G91, T94, V114, I125, V126, T134, G157, L217, S235, G236, V254, V279, V281, L286, V289, I290, V308, L321, I325, D326, L343, F349, S353, I359, I405, L448, Q449, L452, I470, G509, V515, S583, G625, L627, L628 and  
10 A670.

L71, S72, V74, L75, L78, T80, L81, G83, T84, D85, N86, T87, G88, Y89, H90, G91, T94, R95, D96, F97, Y167, F168, H169, H170, N171, G172, D173, I174, S175, N176, D178, D179, R180, Y181, E182, A183, Q184, K186, N187, F188, T189, D190, A192, G193, F194, S195, L196.

15 In a more preferred embodiment, the variant of a maltogenic alpha-amylase comprises one or more substitutions corresponding to the following substitutions in the amino acid sequence set forth in SEQ ID NO: 1:

L217 in combination with L75 (e.g. L217F/Y in combination with L75F/Y), L51W, L75F/Y, L78I, G88A/V/T, G91T/S/V/N, T94V/I/L, V114V/I/L, I125L/M/F/Y/W,  
20 V126I/L, T134V/I/L/M/F/Y/W, G157A/V/I/L, L217V/I/M/F/Y/W, S235I/L/M/F/Y/W, G236A/V/I/L/M/F/Y/W, V254I/L/M/F/Y/W, V279M/I/L/F, V281I/L/M/F/Y/W, L286F, V289I/L/R, I290M/L/F, V308I/L/M/F/Y/W, L321I/M/F/Y/W, I325L/M/F/Y/W, D326E/Q, L343M/F/Y/W, F349W/Y, S353V/I/L, I359L/M/F/Y/W, I405M/L/Y/F/W, L448Y, Q449Y, L452M/Y/F/W, I470M/L/F, G509A/V/I/L/M/S/T/D/N, V515I/L, S583V/I/L/V,  
25 G625A/V/I/L/M/F/Y/W, L627M/F/Y, L628M/I/F/Y/W and A670V/I/L/M/F/Y/W,

L71I, S72C, V74I, L75N/D/Q/I/V, L78N/I, T80I/L/V/S/N/G, L81I/V/S/T/N/Q/K/H, G83A/S/T/N/Q/E/D/R/H/L, T84S/A/N/D/G, D85A/T/S/N/G, N86Q/E/D/Y/H/K, T87S/I, G88A/S/T, Y89F, H90N/Q/K, G91A/S/T, T94N/D/A/M/V/I, R95K/Q, D96N/V/Q/I, F97Y, Y167F/R/C, F168Y, H169N/Q/K, H170N/Q/K, N171D/E/Q/H/R/K/G, G172A/T/S,  
30 D173N/S/T/Y/R/G, I174N/Q/L, S175T/A/N/D, N176S/T/H/Q/P, D178N/Q/E/K/H, D179Y/N/H, R180W, Y181R/F/C/L, E182D, A183S/C/G, Q184E, K186R, N187Q/E/L/F/H/K/V/L, F188Y/L/I/H/N, T189N/D/A/S/H/Y/G, D190E/Q/H/N/K, A192T/D/E/N/K, G193A/S/T, F194Y, S195N/D/E/R/K/G, L196I.

Similar substitutions may be introduced in equivalent positions of other  
35 maltogenic alpha-amylases. Variants of particular interest have a combination of one or more of the above with any of the other modifications disclosed herein.

## **Maltogenic alpha-amylase variants with an altered cleavage pattern**

One aim of the present invention is to change the degradation characteristics of a maltogenic alpha-amylase. Thus, Novamyl hydrolyzes starch to form predominantly maltose (G2) and a small amount of glucose (G1), but virtually no higher  
5 oligosaccharides (G3+). It may be desirable to change this cleavage pattern, e.g. so as to form higher amounts of higher oligosaccharides, such as maltotriose (G3), maltotetraose (G4) and maltopentaose (G5).

A variant of a parent maltogenic alpha-amylase in which the substrate cleavage pattern is altered as compared to said parent may be constructed by a method which  
10 comprises:

- i) identifying the substrate binding area of the parent maltogenic alpha-amylase in a model of the three-dimensional structure, e.g. within a sphere of 4 Å from the substrate binding site as defined in the section above entitled "Substrate Binding Site";
- ii) substituting in the model one or more amino acid residues of the substrate  
15 binding area of the cleft identified in i) which is or are believed to be responsible for the cleavage pattern of the parent with another amino acid residue which from structural or functional considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more amino acid residues of the substrate binding area contemplated to introduce favorable interactions to the substrate or adding one or more  
20 amino acid residues to the substrate binding area contemplated to introduce favorable interactions to the substrate; and
- iii) constructing a maltogenic alpha-amylase variant resulting from step ii) and testing the substrate cleavage pattern of the variant.

Accordingly, another aspect of the invention relates to a variant of a parent  
25 maltogenic alpha-amylase which has an altered substrate binding site as compared to said parent, which variant comprises a modification in a position corresponding to one or both of the following positions in SEQ ID NO: 1:

V281 and/or A629.

In a preferred embodiment, the variant comprises a modification corresponding  
30 to:

V281Q and/or A629N/D/E/Q.

Similar modifications may be introduced in equivalent positions of other maltogenic alpha-amylases. Substitutions of particular interest are any combination of one or both of the above with any of the other modifications disclosed herein.

## **35 Maltogenic alpha-amylase variants with improved ability to reduce retrogradation of starch and/or staling of bread**

The invention provides maltogenic alpha-amylase variants having improved ability to reduce the retrogradation of starch and/or the staling of bread. Preferred

variants comprise a modification at one or more positions corresponding to the following amino acid residues in SEQ ID NO: 1:

A30, K40, N115, T142, F188, T189, P191, A192, G193, F194, S195, D261, N327, K425, K520 and N595.

5. In a more preferred embodiment, the variant comprises one or more modifications corresponding to the following in SEQ ID NO: 1:

A30D, K40R, N115D, T142A, F188L, T189Y,  $\Delta$  (191-195), D261G, D261G, N327S, K425E, K520R and N595I.

### **Determination of residues within 10Å from calcium ions**

- 10 The coordinates of Appendix 1 are read into the INSIGHT program (BIOSYM Technologies). The spatial coordinates are presented showing the bonds between the atoms. The ions are presented as well as the water atoms. The part of the program package for creating subsets was used to create a 10 Å subset around the calcium ions in the structure by using the command ZONE. All residues identified as having an atom
- 15 within the designated 10 Å distance from a calcium ion are compiled and listed by using the command LIST MOLECULE. By giving the ions the name "VAT CA" in the coordinate file, a 10 Å sphere around all atoms called "VAT CA" is compiled. The specific residues identified in this manner are given further above in the section entitled "Calcium binding".

### **20 Determination of cavities**

- The solved structure of Novamyl with the structural coordinates set forth in Appendix 1 reveals many internal crevices and cavities. When analysing for such cavities the Connolly program is normally used (Lee, B. and Richards, F.M. (1971) J. Mol. Biol. 55:379-400). The program uses a probe with radius to search the external
- 25 and internal surface of the protein. The smallest crevice observable in this way has the probe radius.

- To analyse the solved structure a modified version of the Connolly program included in the program of INSIGHT was used. In the first step, the water molecules and the ions were removed by unmerging these atoms from the solved structure. By
- 30 using the command MOLECULE SURFACE SOLVENT the solvent accessible surface area was calculated for all atoms and residues using a probe radius of 1.4 Å, and displayed graphically together with the model of the solved structure. The internal cavities are then seen as dot surfaces with no connections to the external surface.

- Suggestions for specific modifications to fill out the cavities are given above in
- 35 the section entitled "Variants with altered thermostability and/or altered temperature dependent activity profile"). By using the homology built structures or/and comparisons

based on sequence alignment, mutations for homologous structures of maltogenic alpha-amylases can be made.

### **Nomenclature for amino acid modifications**

The nomenclature used herein for defining mutations is essentially as described in WO 92/05249. Thus, F188H indicates a substitution of the amino acid F (Phe) in position 188 with the amino acid H (His). V129S/T/G/V indicates a substitution of V129 with S, T, G or V.  $\Delta$  (191-195) or  $\Delta$  (191-195) indicates a deletion of amino acids in positions 191-195. 192-A-193 indicates an insertion of A between amino acids 192 and 193.

### **10 Polypeptide sequence identity**

For purposes of the present invention, the degree of identity may be suitably determined according to the method described in Needleman, S.B. and Wunsch, C.D., (1970), Journal of Molecular Biology, 48, 443-45, with the following settings for polypeptide sequence comparison: GAP creation penalty of 3.0 and GAP extension penalty of 0.1. The determination may be done by means of a computer program known such as GAP provided in the GCG program package (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711).

The variants of the invention have an amino acid identity with amino acids 1-686 of SEQ ID NO: 1 of at least 70 %, preferably at least 80 %, e.g. at least 90 %, particularly at least 95 % or at least 98 %.

### **Hybridization**

Suitable experimental conditions for determining hybridization between a nucleotide probe and a homologous DNA or RNA sequence involves presoaking of the filter containing the DNA fragments or RNA to hybridize in 5x SSC (sodium chloride/sodium citrate, Sambrook, et al., 1989) for 10 min, and prehybridization of the filter in a solution of 5x SSC, 5x Denhardt's solution (Sambrook, et al., 1989), 0.5% SDS and 100  $\mu$ g/ml of denatured sonicated salmon sperm DNA (Sambrook, et al., 1989), followed by hybridization in the same solution containing a random-primed (Feinberg, A. P. and Vogelstein, B. (1983) *Anal. Biochem.* 132:6-13),  $^{32}$ P-dCTP-labeled (specific activity  $> 1 \times 10^9$  cpm/ $\mu$ g) probe for 12 hours at ca. 45°C. The filter is then washed twice for 30 minutes in 2x SSC, 0.5% SDS at least 55°C (low stringency), preferably at least 60°C (medium stringency), more preferably at least 65°C (medium/high stringency), more preferably at least 70°C (high stringency), even more preferably at least 75°C (very high stringency).

Molecules which hybridize to the oligonucleotide probe under these conditions are detected by exposure to x-ray film.

## Methods of preparing variants of maltogenic alpha-amylases

### Cloning a DNA sequence encoding a Novamyl-like polypeptide

5        The DNA sequence encoding a parent maltogenic alpha-amylase may be isolated from any cell or microorganism producing the maltogenic alpha-amylase in question, using various methods well known in the art, for example, from the *Bacillus* strain NCIB 11837.

10        First, a genomic DNA and/or cDNA library should be constructed using chromosomal DNA or messenger RNA from the organism that produces the maltogenic alpha-amylase to be studied. Then, if the amino acid sequence of the  $\alpha$ -amylase is known, homologous, labelled oligonucleotide probes may be synthesised and used to identify maltogenic alpha-amylase-encoding clones from a genomic library prepared from the organism in question. Alternatively, a labelled oligonucleotide probe containing  
15        sequences homologous to a known  $\alpha$ -amylase gene could be used as a probe to identify maltogenic alpha-amylase-encoding clones, using hybridization and washing conditions of lower stringency.

20        Another method for identifying maltogenic alpha-amylase-encoding clones involves inserting fragments of genomic DNA into an expression vector, such as a plasmid, transforming  $\alpha$ -amylase negative bacteria with the resulting genomic DNA library, and then plating the transformed bacteria onto agar containing a substrate for maltogenic alpha-amylase, thereby allowing clones expressing maltogenic alpha-amylase activity to be identified.

25        Alternatively, the DNA sequence encoding the enzyme may be prepared synthetically by established standard methods, e.g. the phosphoroamidite method described by S.L. Beaucage and M.H. Caruthers (1981) or the method described by Matthes et al. (1984). In the phosphoroamidite method, oligonucleotides are synthesized, e.g. in an automatic DNA synthesizer, purified, annealed, ligated and cloned in appropriate vectors.

30        Finally, the DNA sequence may be of mixed genomic and synthetic origin, mixed synthetic and cDNA origin or mixed genomic and cDNA origin, prepared by ligating fragments of synthetic, genomic or cDNA origin, wherein the fragments correspond to various parts of the entire DNA sequence, in accordance with techniques well known in the art. The DNA sequence may also be prepared by polymerase chain  
35        reaction (PCR) using specific primers, for instance as described in US 4,683,202 or R.K. Saiki et al. (1988).

### Site-directed Mutagenesis

Once a maltogenic alpha-amylase-encoding DNA sequence has been isolated, and desirable sites for modification identified, modifications may be introduced using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired modification sites; mutant nucleotides are inserted during oligonucleotide synthesis. In a specific method, a single-stranded gap of DNA, bridging the maltogenic alpha-amylase-encoding sequence, is created in a vector carrying the maltogenic alpha-amylase gene. Then the synthetic nucleotide, bearing the desired modification, is annealed to a homologous portion of the single-stranded DNA. The remaining gap is then filled in with DNA polymerase I (Klenow fragment) and the construct is ligated using T4 ligase. A specific example of this method is described in Morinaga et al. (1984). US 4,760,025 discloses the introduction of oligonucleotides encoding multiple modifications by performing minor alterations of the cassette. However, an even greater variety of modifications can be introduced at any one time by the Morinaga method because a multitude of oligonucleotides, of various lengths, can be introduced.

Another method of introducing modifications into a maltogenic alpha-amylase-encoding DNA sequences is described in Nelson and Long (1989). It involves a 3-step generation of a PCR fragment containing the desired modification introduced by using a chemically synthesized DNA strand as one of the primers in the PCR reactions. From the PCR-generated fragment, a DNA fragment carrying the modification may be isolated by cleavage with restriction endonucleases and reinserted into an expression plasmid.

### Random Mutagenesis

Random mutagenesis is suitably performed either as localised or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

The random mutagenesis of a DNA sequence encoding a parent maltogenic alpha-amylase may be conveniently performed by use of any method known in the art.

In relation to the above, a further aspect of the present invention relates to a method for generating a variant of a parent Novamyl-like  $\alpha$ -amylase, wherein the variant exhibits increased stability at low pH and at low calcium concentration relative to the parent, the method comprising:

- (a) subjecting a DNA sequence encoding the parent Novamyl-like  $\alpha$ -amylase to random mutagenesis,
- (b) expressing the mutated DNA sequence obtained in step (a) in a host cell, and

(c) screening for host cells expressing a Novamyl-like  $\alpha$ -amylase variant which has an altered property relative to the parent Novamyl-like  $\alpha$ -amylase.

Step (a) of the above method of the invention is preferably performed using doped primers, as described in the working examples herein (*vide infra*).

- 5 For instance, the random mutagenesis may be performed by use of a suitable physical or chemical mutagenizing agent, by use of a suitable oligonucleotide, or by subjecting the DNA sequence to PCR generated mutagenesis. Furthermore, the random mutagenesis may be performed by use of any combination of these mutagenizing agents. The mutagenizing agent may, e.g., be one which induces transitions,  
10 transversions, inversions, scrambling, deletions, and/or insertions.

Examples of a physical or chemical mutagenizing agent suitable for the present purpose include ultraviolet (UV) irradiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine (MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide analogues. When  
15 such agents are used, the mutagenesis is typically performed by incubating the DNA sequence encoding the parent enzyme to be mutagenized in the presence of the mutagenizing agent of choice under suitable conditions for the mutagenesis to take place, and selecting for mutated DNA having the desired properties.

When the mutagenesis is performed by the use of an oligonucleotide, the  
20 oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleotide at the positions which are to be changed. The doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide can be incorporated into the DNA encoding the maltogenic alpha-amylase enzyme by any published technique, using e.g. PCR, LCR  
25 or any DNA polymerase and ligase as deemed appropriate.

Preferably, the doping is carried out using "constant random doping", in which the percentage of wild-type and modification in each position is predefined. Furthermore, the doping may be directed toward a preference for the introduction of certain nucleotides, and thereby a preference for the introduction of one or more  
30 specific amino acid residues. The doping may be made, e.g., so as to allow for the introduction of 90% wild type and 10% modifications in each position. An additional consideration in the choice of a doping scheme is based on genetic as well as protein-structural constraints. The doping scheme may be made by using the DOPE program which, *inter alia*, ensures that introduction of stop codons is avoided.

35 When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent maltogenic alpha-amylase enzyme is subjected to PCR under conditions that increase the misincorporation of nucleotides (Deshler 1992; Leung et al., Technique, Vol.1, 1989, pp. 11-15).



A mutator strain of *E. coli* (Fowler et al., Molec. Gen. Genet., 133, 1974, pp. 179-191), *S. cerevisiae* or any other microbial organism may be used for the random mutagenesis of the DNA encoding the maltogenic alpha-amylase by, e.g., transforming a plasmid containing the parent enzyme into the mutator strain, growing the mutator strain with the plasmid and isolating the mutated plasmid from the mutator strain. The mutated plasmid may be subsequently transformed into the expression organism.

The DNA sequence to be mutagenized may be conveniently present in a genomic or cDNA library prepared from an organism expressing the parent maltogenic alpha-amylase. Alternatively, the DNA sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenising agent. The DNA to be mutagenized may also be present in a host cell either by being integrated in the genome of said cell or by being present on a vector harbored in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

In some cases it may be convenient to amplify the mutated DNA sequence prior to performing the expression step b) or the screening step c). Such amplification may be performed in accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

Subsequent to the incubation with or exposure to the mutagenising agent, the mutated DNA is expressed by culturing a suitable host cell carrying the DNA sequence under conditions allowing expression to take place. The host cell used for this purpose may be one which has been transformed with the mutated DNA sequence, optionally present on a vector, or one which was carried the DNA sequence encoding the parent enzyme during the mutagenesis treatment. Examples of suitable host cells are the following: gram positive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, *Streptomyces lividans* or *Streptomyces murinus*; and gram negative bacteria such as *E. coli*.

The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

#### Localized random mutagenesis

The random mutagenesis may be advantageously localized to a part of the parent maltogenic alpha-amylase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular importance for a given property of the enzyme, and when modified are expected to result in a variant

having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

5 The localized, or region-specific, random mutagenesis is conveniently performed by use of PCR generated mutagenesis techniques as described above or any other suitable technique known in the art. Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g., by insertion into a suitable vector, and said part may be subsequently subjected to mutagenesis by use of any of the mutagenesis methods discussed above.

10 For region-specific random mutagenesis with a view to improving the stability of calcium binding of a parent maltogenic alpha-amylase, codon positions corresponding to the following amino acid residues from the amino acid sequence set forth in SEQ ID NO: 1 may appropriately be targeted:

Residues:Regions:

15 16-33, 35-36, 40: 16-40  
46-54, 56: 46-56  
73-81: 73-81  
87-89, 91, 93-96, 99-105, 109: 87-109  
129-134, (145, 150): 129-134  
20 167-172, 174, 177, 180-189: 167-189  
196-202, 206-210: 196-210  
228-235, 237: 228-237  
378  
637

25 With a view to achieving improved binding of a substrate, i.e., improved binding of a carbohydrate species, such as amylose or amylopectin, by a maltogenic alpha-amylase variant with a modified, e.g. higher, substrate specificity and/or a modified, e.g. higher, specificity with respect to cleavage, i.e. hydrolysis, of the substrate, it appears that the following codon positions in the following regions of the amino acid sequence  
30 shown in SEQ ID NO: 1, may particularly appropriately be targeted for modification by region-specific mutagenesis:

70-97, 127-143, 174-198, 226-233, 255-270, 282-292, 324-331, 370-376.

For region-specific random mutagenesis with a view to altering the substrate specificity and/or the pH dependent activity profile, the following regions of SEQ ID NO:  
35 1 may be targeted: 70-97, 174-198.

For random mutagenesis with a view to improving the thermostability, the residues and regions described above may be targeted, particularly those described for altering stability, filling internal holes, improved Ca binding, interdomain and intradomain contacts, helix capping, proline substitution, and histidine substitution. In

addition, the following regions may be targeted with a view to improving the thermostability: 70-109, 167-200. Also, any amino acid residue which is substituted in a variant having improved thermostability may be targeted, e.g. those in the following positions: 115, 342, 387, 422, 425, 483, 520, 594 and 600.

5 General method for random mutagenesis by use of the DOPE program

The random mutagenesis may be carried out by the following steps:

1. Select regions of interest for modification in the parent enzyme
2. Decide on mutation sites and non-mutated sites in the selected region
3. Decide on which kind of mutations should be carried out, e.g. with respect to  
10 the desired stability and/or performance of the variant to be constructed
4. Select structurally reasonable mutations
5. Adjust the residues selected by step 3 with regard to step 4.
6. Analyse by use of a suitable dope algorithm the nucleotide distribution.
7. If necessary, adjust the wanted residues to genetic code realism, e.g. taking  
15 into account constraints resulting from the genetic code, e.g. in order to avoid introduction of stop codons; the skilled person will be aware that some codon combinations cannot be used in practice and will need to be adapted
8. Make primers
9. Perform random mutagenesis by use of the primers
- 20 10. Select resulting  $\alpha$ -amylase variants by screening for the desired improved properties.

Suitable dope algorithms for use in step 6 are well known in the art. One such algorithm is described by Tomandl, D. et al., 1997, Journal of Computer-Aided Molecular Design 11:29-38. Another algorithm is DOPE (Jensen, LJ, Andersen, KV,  
25 Svendsen, A, and Kretzschmar, T (1998) Nucleic Acids Research 26:697-702).

**Expression of maltogenic alpha-amylase variants**

The construction of the variant of interest is accomplished by cultivating a microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing the variant, and optionally subsequently recovering  
30 the variant from the resulting culture broth. This is described in detail further below.

According to the invention, a DNA sequence encoding the variant produced by methods described above, or by any alternative methods known in the art, can be expressed, in the form of a protein or polypeptide, using an expression vector which typically includes control sequences encoding a promoter, operator, ribosome binding  
35 site, translation initiation signal, and, optionally, a repressor gene or various activator genes.

The recombinant expression vector carrying the DNA sequence encoding an maltogenic alpha-amylase variant of the invention may be any vector which may conveniently be subjected to recombinant DNA procedures, and the choice of vector will often depend on the host cell into which it is to be introduced. Thus, the vector may  
5 be an autonomously replicating vector, i.e. a vector which exists as an extrachromosomal entity, the replication of which is independent of chromosomal replication, e.g. a plasmid, a bacteriophage or an extrachromosomal element, minichromosome or an artificial chromosome. Alternatively, the vector may be one which, when introduced into a host cell, is integrated into the host cell genome and replicated together with the  
10 chromosome(s) into which it has been integrated.

In the vector, the DNA sequence should be operably connected to a suitable promoter sequence. The promoter may be any DNA sequence which shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell. Examples of suitable pro-  
15 moters for directing the transcription of the DNA sequence encoding a maltogenic alpha-amylase variant of the invention, especially in a bacterial host, are the promoter of the *lac* operon of *E. coli*, the *Streptomyces coelicolor* agarase gene *dagA* promoters, the promoters of the *Bacillus licheniformis*  $\alpha$ -amylase gene (*amyL*), the promoters of the *Bacillus stearothermophilus* maltogenic amylase gene (*amyM*), the promoters of the  
20 *Bacillus amyloliquefaciens*  $\alpha$ -amylase (*amyQ*), the promoters of the *Bacillus subtilis* *xylA* and *xylB* genes, etc. For transcription in a fungal host, examples of useful promoters are those derived from the gene encoding *A. oryzae* Taka amylase, *Rhizomucor miehei* aspartic proteinase, *A. niger* neutral  $\alpha$ -amylase, *A. niger* acid stable  $\alpha$ -amylase, *A. niger* glucoamylase, *Rhizomucor miehei* lipase, *A. oryzae* alkaline protease, *A.*  
25 *oryzae* triose phosphate isomerase or *A. nidulans* acetamidase.

The expression vector of the invention may also comprise a suitable transcription terminator and, in eukaryotes, polyadenylation sequences operably connected to the DNA sequence encoding the maltogenic alpha-amylase variant of the invention. Termination and polyadenylation sequences may suitably be derived from  
30 the same sources as the promoter.

The vector may further comprise a DNA sequence enabling the vector to replicate in the host cell in question. Examples of such sequences are the origins of replication of plasmids pUC19, pACYC177, pUB110, pE194, pAMB1 and pIJ702.

The vector may also comprise a selectable marker, e.g. a gene the product of  
35 which complements a defect in the host cell, such as the *dal* genes from *B. subtilis* or *B. licheniformis*, or one which confers antibiotic resistance such as ampicillin, kanamycin, chloramphenicol or tetracycline resistance. Furthermore, the vector may comprise *Aspergillus* selection markers such as *amdS*, *argB*, *niaD* and *sC*, a marker

giving rise to hygromycin resistance, or the selection may be accomplished by co-transformation, e.g. as described in WO 91/17243.

While intracellular expression may be advantageous in some respects, e.g. when using certain bacteria as host cells, it is generally preferred that the expression is  
5 extracellular. In general, the *Bacillus*  $\alpha$ -amylases mentioned herein comprise a preregion permitting secretion of the expressed protease into the culture medium. If desirable, this preregion may be replaced by a different preregion or signal sequence, conveniently accomplished by substitution of the DNA sequences encoding the respective preregions.

10 The procedures used to ligate the DNA construct of the invention encoding maltogenic alpha-amylase variant, the promoter, terminator and other elements, respectively, and to insert them into suitable vectors containing the information necessary for replication, are well known to persons skilled in the art (cf., for instance, Sambrook et al. (1989)).

15 The cell of the invention, either comprising a DNA construct or an expression vector of the invention as defined above, is advantageously used as a host cell in the recombinant production of a maltogenic alpha-amylase variant of the invention. The cell may be transformed with the DNA construct of the invention encoding the variant, conveniently by integrating the DNA construct (in one or more copies) in the host  
20 chromosome. This integration is generally considered to be an advantage as the DNA sequence is more likely to be stably maintained in the cell. Integration of the DNA constructs into the host chromosome may be performed according to conventional methods, e.g. by homologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in connection with  
25 the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mammal or an insect, but is preferably a microbial cell, e.g. a bacterial or a fungal (including yeast) cell.

Examples of suitable bacteria are gram positive bacteria such as *Bacillus*  
30 *subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, or *Streptomyces lividans* or *Streptomyces murinus*, or gram negative bacteria such as *E.coli*. The transformation of the bacteria may, for instance, be effected by protoplast transformation or  
35 by using competent cells in a manner known *per se*.

The yeast organism may favourably be selected from a species of *Saccharomyces* or *Schizosaccharomyces*, e.g. *Saccharomyces cerevisiae*. The filamentous fungus may advantageously belong to a species of *Aspergillus*, e.g. *Aspergillus oryzae* or *Aspergillus niger*. Fungal cells may be transformed by a process

involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall in a manner known *per se*. A suitable procedure for transformation of *Aspergillus* host cells is described in EP 238 023.

In a yet further aspect, the present invention relates to a method of producing a  
5 maltogenic alpha-amylase variant of the invention, which method comprises cultivating a host cell as described above under conditions conducive to the production of the variant and recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and obtaining expression of the maltogenic  
10 alpha-amylase variant of the invention. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

The maltogenic alpha-amylase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including  
15 separating the cells from the medium by centrifugation or filtration, and precipitating proteinaceous components of the medium by means of a salt such as ammonium sulfate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

### Testing of maltogenic alpha-amylase variants

20 Maltogenic alpha-amylase variants produced by any of the methods described above may be tested, either prior to or after purification, for amylolytic activity in a screening assay which measures the ability of the variant to degrade starch. The screening in step 10 in the above-mentioned random mutagenesis method of the invention may be conveniently performed by use of a filter assay based on the following  
25 procedure: A microorganism capable of expressing the mutated maltogenic alpha-amylase of interest is incubated on a suitable medium and under suitable conditions for secretion of the enzyme, the medium being covered with two filters comprising a protein-binding filter placed under a second filter exhibiting a low protein binding capability. The microorganism is grown on the second, top filter. Subsequent to the  
30 incubation, the bottom protein-binding filter comprising enzymes secreted from the microorganism is separated from the second filter comprising the microorganism. The protein-binding filter is then subjected to screening for the desired enzymatic activity, and the corresponding microbial colonies present on the second filter are identified. The first filter used for binding the enzymatic activity may be any protein-binding filter,  
35 e.g., nylon or nitrocellulose. The second filter carrying the colonies of the expression organism may be any filter that has no or low affinity for binding proteins, e.g., cellulose acetate or Durapore™.

Screening consists of treating the first filter to which the secreted protein is bound with a substrate that allows detection of the  $\alpha$ -amylase activity. The enzymatic activity may be detected by a dye, fluorescence, precipitation, pH indicator, IR-absorbance or any other known technique for detection of enzymatic activity. The  
5 detecting compound may be immobilized by any immobilizing agent e.g. agarose, agar, gelatine, polyacrylamide, starch, filter paper, cloth; or any combination of immobilizing agents. For example,  $\alpha$ -amylase activity can be detected by Cibacron Red labelled amylopectin, which is immobilized in agarose.  $\alpha$ -amylase activity on this substrate produces zones on the plate with reduced red color intensity.

10 To screen for variants with increased stability, the filter with bound maltogenic alpha-amylase variants can be pretreated prior to the detection step described above to inactivate variants that do not have improved stability relative to the parent maltogenic alpha-amylase. This inactivation step may consist of, but is not limited to, incubation at  
15 elevated temperatures in the presence of a buffered solution at any pH from pH 2 to 12, and/or in a buffer containing another compound known or thought to contribute to altered stability e.g., surfactants, EDTA, EGTA, wheat flour components, or any other relevant additives. Filters so treated for a specified time are then rinsed briefly in deionized water and placed on plates for activity detection as described above. The conditions are chosen such that stabilized variants show increased enzymatic activity  
20 relative to the parent after incubation on the detection media.

To screen for variants with altered thermostability, filters with bound variants are incubated in buffer at a given pH (e.g., in the range from pH 2-12) at an elevated temperature (e.g., in the range from 50°-110°C) for a time period (e.g., from 1-20  
25 minutes) to inactivate nearly all of the parent maltogenic alpha-amylase, rinsed in water, then placed directly on a detection plate containing immobilized Cibacron Red labelled amylopectin and incubated until activity is detectable. Similarly, pH dependent stability can be screened for by adjusting the pH of the buffer in the above inactivation step such that the parent maltogenic alpha-amylase is inactivated, thereby allowing detection of only those variants with increased stability at the pH in question. To screen  
30 for variants with increased calcium-dependent stability calcium chelators, such as ethylene glycol-bis( $\beta$ -aminoethyl ether) N,N,N',N'-tetraacetic acid (EGTA), is added to the inactivation buffer at a concentration such that the parent maltogenic alpha-amylase is inactivated under conditions further defined, such as buffer pH, temperature or a specified length of incubation.

35 The variants of the invention may be suitably tested by assaying the starch-degrading activity of the variant, for instance by growing host cells transformed with a DNA sequence encoding a variant on a starch-containing agarose plate and identifying starch-degrading host cells as described above. Further testing in regard to altered properties, including specific activity, substrate specificity, cleavage pattern,

thermoactivation, thermostability, pH dependent activity or optimum, pH dependent stability, temperature dependent activity or optimum, transglycosylation activity, stability, and any other parameter of interest, may be performed on purified variants in accordance with methods known in the art as described below.

#### 5 Degradation of $\beta$ -limit dextrin by maltogenic alpha-amylase:

Another important parameter in the evaluation of the substrate specificity of maltogenic alpha-amylase variants may be the degree to which such enzymes are capable of degrading starch that has been exhaustively treated with the exoglycosylase  $\beta$ -amylase. To screen for variants which show patterns of degradation on such a  
 10 substrate differing from the patterns produced by the parent maltogenic alpha-amylase the following assay is performed:  $\beta$ -limit dextrin is prepared by incubating 25 ml 1% amylopectin in McIlvane buffer (48.5 mM citrate and 193 mM sodium phosphate pH 5.0) with 24  $\mu$ g/ml  $\beta$ -amylase overnight at 30°C. Unhydrolysed amylopectin (i.e.,  $\beta$ -limit dextrin) is precipitated with 1 volume 98% ethanol, washed and redissolved in water. 1  
 15 ml  $\beta$ -limit dextrin is incubated with 18  $\mu$ l enzymes (at 2.2 mg/ml) and 100  $\mu$ l 0.2 M citrate-phosphate pH 5.0 for 2 hrs at 30°C and analysed by HPLC as described above. Total hydrolysis of  $\beta$ -limit dextrin is carried out in 2M HCl at 95°C. The concentration of reducing ends is measured by methods known in the art.

#### Calcium binding affinity

20 Unfolding of maltogenic alpha-amylases by exposure to heat or to denaturants such as guanidine hydrochloride is accompanied by a decrease in fluorescence, and loss of calcium ions leads to unfolding. Thus, the affinity of a maltogenic alpha-amylase variant for calcium can be measured by fluorescence measurements before and after incubation of the variant (e.g., at a concentration of 10 mg/ml) in a buffer (e.g., 50 mM  
 25 HEPES, pH 7) with different concentrations of calcium (e.g., in the range from 1 mM-100 mM) or of EGTA (e.g., in the range from 1-1000 mM) for a sufficiently long period of time (such as 22 hours at 55°C).

The measured fluorescence,  $F$ , is composed of contributions from the folded and unfolded forms of the enzyme. The following equation can be derived to describe  
 30 the dependence of  $F$  on calcium concentration ( $[Ca]$ ):

$$F = [Ca]/(K_{diss} + [Ca])(a_N - b_N \log([Ca])) + K_{diss}/(K_{diss} + [Ca])(a_U - b_U \log([Ca]))$$

where  $a_N$  is the fluorescence of the native (folded) form of the enzyme,  $b_N$  is the linear dependence of  $a_N$  on the logarithm of the calcium concentration (as observed  
 35 experimentally),  $a_U$  is the fluorescence of the unfolded form and  $b_U$  is the linear dependence of  $a_U$  on the logarithm of the calcium concentration.  $K_{diss}$  is the apparent calcium binding constant for an equilibrium process as follows:



$K_{\text{diss}}$

$N \rightleftharpoons U + Ca$  (N = native enzyme; U = unfolded enzyme)

In fact, unfolding proceeds extremely slowly and is irreversible. The rate of unfolding is dependent on calcium concentration, and such dependency for a given enzyme provides a measure of the calcium binding affinity of the enzyme. By defining a standard set of reaction conditions (e.g., 22 hours at 55°C), a meaningful comparison of  $K_{\text{diss}}$  for different maltogenic alpha-amylase variants can be made.

### Industrial Applications

The maltogenic alpha-amylase variants of the invention possesses valuable properties which may be advantageously used in various industrial applications. In particular, the enzyme finds potential application for retarding or preventing retrogradation, and thus the staling, of starch based food such as common in the baking industry.

The variant may be used for the preparation of bread and other bread products in accordance with conventional techniques known in the art.

It is believed that the modification of the starch fraction by use of the present invention results in increased volume in baked products and improved organoleptic qualities, such as flavour, mouth feel, palatability, aroma and crust colour.

The maltogenic alpha-amylase variant may be used as the only enzyme or as a major enzymatic activity in combination with one or more additional enzymes, such as xylanase, lipase, glucose oxidase and other oxidoreductases, or an amylolytic enzyme.

The enzyme variants of the invention also find industrial applicability as a component in washing, dishwashing and hard-surface cleaning detergent compositions. Some variants are particularly useful in a process for the manufacture of linear oligosaccharides, or in the production of sweeteners and ethanol from starch, and/or for textile desizing. Conditions for conventional starch conversion processes, including starch liquefaction and/or saccharification processes, are described in, e.g., US 3,912,590 and in EP patent publications Nos. 252,730 and 63,909.

The invention is further illustrated with reference to the following examples which are not intended to be in any way limiting to the scope of the invention as claimed.

### Determination of maltogenic amylase in MANU

One Maltogenic Amylase Novo Unit (MANU) is the amount of enzyme which under standard will cleave one  $\mu\text{mol}$  maltotriose per minute. The standard conditions are 10 mg/ml maltotriose, 37°C, pH 5.0, 30 minutes reaction time.

The pH dependence is found by repeating this measurement at the same conditions, but at different pH values.

## EXAMPLES

### Example 1: Construction of a variant of Novamyl with altered pH dependent activity

Novamyl is expressed in *Bacillus subtilis* from a plasmid denoted herein as pLBei010. This plasmid contains *amyM* in which the expression of *amyM* is directed by its own promoter and the complete gene encoding Novamyl, e.g., as contained in the strain DSM 11837. The plasmid contains the origin of replication, *ori*, from plasmid pUB110 and an kanamycin resistance marker for selection purposes. pLBei010 is shown in Fig. 1.

#### 10 Primer sequences

Site directed mutants of Novamyl were constructed by the megaprimer method essentially as described by Kammann et al. (1989). Briefly, a mutagenic oligonucleotide primer is used together in a PCR reaction with a suitable opposite DNA strand end primer to create a preliminary PCR product. This product is then used as a megaprimer together with another opposite DNA strand end primer to create a double-stranded DNA product. The product of the final PCR reaction was routinely used to replace a corresponding DNA fragment in the pLBei010 plasmid by standard cloning procedures. Mutants were transformed directly into *Bacillus subtilis* strain SHa273, a derivative of *Bacillus subtilis* 168 which is *apr*<sup>-</sup>, *npr*<sup>-</sup>, *amyE*<sup>-</sup>, *amyR2*<sup>-</sup> and prepared by methods known in the art.

Oligonucleotide primers used in the construction of described variants are as listed below:

#### Variant Sequence (5' → 3')

F188H: SEQ ID NO: 3

25 F188E: SEQ ID NO: 4

F284E: SEQ ID NO: 5

F284D: SEQ ID NO: 6

F284K: SEQ ID NO: 7

N327D: SEQ ID NO: 8

30 Variant Sequence (3' → 5')

T288K: SEQ ID NO: 9

T288R: SEQ ID NO: 10

Aspartate variants of F284, T288 and N327 were obtained using primer A189 (SEQ ID NO: 11) and B649 (SEQ ID NO: 12) as end-primers.

35 F188-variants F188L, T189Y were obtained using primer A82 (SEQ ID NO: 13) and B346 (SEQ ID NO: 14) as end-primers.

PCR products with the desired modification(s) were purified, digested with appropriate enzymes, separated by agarose gel electrophoresis and extracted, ethanol precipitated in the presence of glycogen, resuspended in H<sub>2</sub>O, ligated to pLBei010 which had been digested with the same appropriate enzymes, and transformed into  
5 *Bacillus subtilis* SHa273. Transformants were checked for size by colony PCR and for the insertion or removal of specific restriction sites by restriction enzyme digestion. Positive colonies were verified by DNA sequencing methods as described in the art.

### Fermentation

The *B. subtilis* SHa273 mutant clones were grown overnight on LB-Kana (10  
10 µg/ml)-Starch plates at 37°C. The colonies from the plate were resuspended in 10 ml Luria broth. One-sixth of each of the suspensions were inoculated into a 500 ml shake flasks containing 100 ml PS-1 media, a soy meal/sucrose-based media, kanamycin for a final concentration of 10 µg/ml and 100 µl 5M NaOH. The pH was adjusted to 7.5 with NaOH before inoculation. The cultures were incubated for five days at 30°C with  
15 shaking at 270-300 rpm.

### Enzyme Purification

Large particles from the media were removed by flocculation before affinity chromatography. Superfloc C521 (American Cyanmide Company) was used as the cationic flocculant and Superfloc A130 (American Cyanmide Company) as the anionic  
20 flocculant.

The culture suspension was diluted 1:1 with deionized water and the pH was adjusted to approx. 7.5. A volume of 0.01 ml of 50% w/w CaCl<sub>2</sub> per ml diluted culture was added during stirring. A volume of 0.015 ml of 20% w/w Na-aluminate per ml diluted culture was titrated with 20% formic acid, while keeping the pH between 7 and 8. While  
25 stirring 0.025 ml 10% v/v of C521 per ml diluted culture was added, followed by 0.05 ml 1% v/v A130 per ml diluted culture, or until flocculation was observed. The solution was centrifuged at 4500 rpm for 30 minutes. Filtration was performed using a filter of pore size of 0.45 µm to exclude larger particles and any remaining bacteria. The filtered solution was stored at -20°C.

### 30 Immobilization of α-cyclodextrin to DSV-agarose

One hundred mg of α-cyclodextrin of molecular weight 972.86g/mol (Fluka 28705) was dissolved in 20 ml coupling buffer (0.5M Na<sub>2</sub>CO<sub>3</sub>, pH 11). Ten ml of DSV-agarose (Mini-Leak, Medium 10-20 mmol/l of divinyl sulfone activated agarose (Kem-En-Tec) was washed thoroughly with deionized water, then dried by suction and  
35 transferred to the α-cyclodextrin solution. After the mixture had stirred for 24 hr at ambient temperature, the gel was washed with deionized water, followed by 0.5M

KHCO<sub>3</sub>. The gel was transferred to the blocking buffer (20ml 0.5M KHCO<sub>3</sub> + 1ml mercaptoethanol), stirred for 2 hr at ambient temperature, then washed with deionized water.

#### Affinity chromatography

- 5 The variants were purified by affinity chromatography using the Pharmacia FPLC System. A 0.04 volume of 1M Na-acetate pH 5 was added to the filtrate obtained by flocculation to adjust pH and CaCl<sub>2</sub> was added to a final concentration of 10<sup>-10</sup> M. The solution was filtered and degassed. A Pharmacia XK16 column was prepared with ten ml of the immobilised  $\alpha$ -cyclodextrin, then equilibrated in the equilibration buffer (25
- 10 mM Na-acetate pH 5) by washing with approximately 10 times the column volume. The filtrate was applied to the XK16 column, which was then washed with the equilibration buffer until protein could no longer be detected in the washing buffer. The column was washed with the equilibration buffer containing 0.5M NaCl to elute nonspecific material, followed by another wash with 2-3 times the column volume of the equilibration buffer.
- 15 All washings were performed using a flow rate of 10ml/min. Specifically bound material was eluted using a solution of 2%  $\alpha$ -cyclodextrin in the wash buffer and collected using the Pharmacia Liquid Chromatography Collector LCC-500 Plus using a flow rate of 5 ml/min.

#### **Example 2: pH dependent activity of variants**

- 20 The variants prepared in the preceding Example were tested for activity at various pH values as follows.

A colorimetric glucose oxidase-peroxidase assay for liberated glucose from maltotriose or amylopectin was used to determine the pH activity profiles of the enzyme variants (Glucose/GOD-Perid<sup>®</sup> Method, Boehringer Mannheim, Indianapolis IN). Activity

25 was assayed in a buffer of 25 mM citrate-phosphate, 0.1mM CaCl<sub>2</sub> at pH values of 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8 and 8.6. The buffer pH was adjusted using NaOH and enzymes were diluted in 25 mM citrate-phosphate buffer pH 5. Measurements were taken in duplicate to obtain an average value. All values are relative to the pH at which the highest level of activity is seen.

- 30 The results, shown in the table below, indicate that each of the variants has an alteration in the pH dependent activity profile when compared to the parent Novamyl<sup>®</sup>. The highest level of activity for each variant is designated 100% and the activity of that variant measured at the other indicated pH values is a relative percentage of that maximum.

35

| Modifications | pH |
|---------------|----|
|---------------|----|

|               | 2.0 | 2.5 | 3.0 | 3.5 | 4.0 | 4.5 | 5.0 | 5.5 | 6.0 | 6.5 | 7.0 | 7.5 | 8.0 | 8.6 |
|---------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| None (parent) | 0   | 0   | 0   | 8   | 47  | 80  | 100 | 95  | 91  | 80  | 66  | 39  | 35  | 30  |
| F188H         | 1   | 0   | 0   | 1   | 3   | 29  | 77  | 99  | 100 | 88  | 59  | 39  | 31  | 27  |
| F188E         | 0   | 0   | 0   | 2   | 27  | 62  | 89  | 100 | 93  | 71  | 46  | 28  | 20  | 18  |
| T288R         | 0   | 0   | 0   | 8   | 51  | 77  | 94  | 100 | 86  | 73  | 50  | 34  | 27  | 12  |
| N327D         | 1   | 1   | 7   | 27  | 67  | 95  | 100 | 98  | 77  | 33  | 19  | 11  | 5   | 0   |

Further, a number of Novamyl variants were tested for activity at pH 4.0 and 5.0, taking the activity of Novamyl at the same pH as 100 %. The activity was determined by hydrolysis of maltotriose (10 mg/ml) at 60°C, 50 mM sodium acetate, 1 mM CaCl<sub>2</sub>. The results are expressed as the ratio between activity at pH 5.0 and pH 4.0:

| Modifications                 | pH 5.0/pH 4.0 |
|-------------------------------|---------------|
| N131D                         | 0.24          |
| I174Q                         | 0.31          |
| G397P                         | 0.40          |
| H103Y                         | 0.40          |
| Δ 262-266                     | 0.47          |
| T142A + D261G + T288P + Q449R | 0.50          |
| S32Q                          | 0.53          |
| S32D                          | 0.55          |
| T142A+ D261G                  | 0.62          |
| G370N+ N371G                  | 0.66          |
| S32N                          | 0.68          |
| N176S                         | 0.79          |
| D17E                          | 0.80          |
| None (parent)                 | 1             |
| Δ 191                         | 1.39          |
| 192-A-193                     | 1.61          |
| I174E                         | 1.80          |
| 192-A-G-193                   | 1.90          |
| Δ 192                         | 2.22          |

F188L + D261G + T288P

2.47

The results demonstrate that variants with a higher or lower pH optimum can be obtained according to the invention.

### Example 3: Thermostability of variants

#### 5 Incubation at 80°C

The thermostability of a number of Novamyl variants was tested by incubating an aqueous solution at 80 C, pH 4.3, 50 mM acetate buffer, 1mM CaCl<sub>2</sub>, and measuring the residual amylase activity at various times. The parent enzyme, Novamyl, was included for comparison. The results are expressed as residual activity at various 10 times in percent of initial activity:

| Variant                              | 0   | 5 min. | 10 min. | 15 min. | 20 min. | 25 min. |
|--------------------------------------|-----|--------|---------|---------|---------|---------|
| None (parent)                        | 100 | 23     | 9       | 3       | 1       | 0       |
| A197P + D261G + T288P<br>+ N342S     | 100 | 36     | 28      | 14      | 16      | 9       |
| A30D+ K40R+ D261G<br>T288K           | 100 | 38     | 24      | 15      | 13      | 10      |
| T142A+ N327S+ K425E+<br>K520R+ N595I | 100 | 64     | 31      | 18      | 7       | 4       |
| T142A + D261G + T288P<br>+ Q449R     | 100 | 47     | 39      | 25      | 19      | 11      |
| T142A + D261G + T288P<br>+ Q449R     | 100 | 45     | 36      | 27      | 16      | 9       |
| K40R+ F188L+ D261G+<br>A483T         | 100 | 56     | 48      | 40      | 36      | 30      |
| F188L+ V336L+ T525A                  | 100 | 63     | 49      | 48      | 52      | 47      |
| F188I+ Y422F+ I660V                  | 100 | 71     | 60      | 51      | 43      | 38      |
| N115D+ F188L                         | 100 | 73     | 60      | 51      | 44      | 39      |
| F188L+ D261G+ T288P                  | 100 | 60     | 67      | 66      | 63      | 67      |
| F188L + D261G + T288P<br>+ A483T     | 100 | 66     | 72      | 73      | 75      | 78      |
| N26S + F188L + D261G +               | 100 | 80     | 80      | 82      | 84      | 84      |

|  |     |    |    |    |    |    |
|--|-----|----|----|----|----|----|
| <b>T288P + T594A + I600V</b>                           |     |    |    |    |    |    |
| <b>N26S + T80A + F188L +<br/>D261G + T288P + R291L</b> | 100 | 80 | 75 | 82 | 83 | 87 |

The above data show a clearly improved thermostability for the variants compared to the parent amylase. Thus, after 15 minutes incubation at 80 C, a number of variants show at least 25 % residual activity, and some even show at least 50 % residual activity, whereas the parent enzyme has essentially lost its activity.

#### Incubation at 85°C

The Novamyl variant S32E was tested by incubation with 1 mM Ca<sup>++</sup> at 85°C for 15 minutes. The variant showed a residual activity of 48 % whereas the parent enzyme (Novamyl) showed 32 % residual activity at the same conditions.

#### 10 Incubation at 90°C

Four variants and the parent enzyme were tested by incubating at 90°C, pH 5.0, 50 mM acetate buffer, 1 mM CaCl<sub>2</sub>, and measuring the residual activity. The results were as follows:

| <b>Variant</b>  | <b>0</b> | <b>10 min.</b> | <b>20 min.</b> | <b>30 min.</b> |
|---|----------|----------------|----------------|----------------|
| <b>None (parent)</b>                                    | 100      | 5              | 0              | 0              |
| <b>F188L + D261G + T288P</b>                            | 100      | 70             | 41             | 28             |
| <b>N26S + F188L + D261G + T288P + T594A +<br/>I600V</b> | 100      | 71             | 54             | 39             |
| <b>N26S + T80A + F188L + D261G + T288P +<br/>R291L</b>  | 100      | 43             | 26             | 13             |
| <b>F188L + D261G + T288P + A483T</b>                    | 100      | 54             | 39             | 26             |

15 The variants show a clearly improved thermostability. Thus, the variants retain more than 10 % (or even more than 20 %) relative activity after 30 minutes incubation at 90°C, whereas the parent enzyme loses all activity after 20 minutes.

#### DSC

20 Further, the thermostability was tested for some Novamyl variants by DSC (differential scanning calorimetry) at pH values in the range 4.0-5.5. Again, the parent amylase was included for comparison. The results are expressed as the denaturation temperature (T<sub>m</sub>) at the given pH:

| Modifications                     | pH 4.0 | pH 4.3 | pH 5.0 | pH 5.5 |
|-----------------------------------|--------|--------|--------|--------|
| None (parent)                     | 64 C   | 79 C   | 83 C   | 88 C   |
| N115D+ F188L                      |        | 86 C   |        | 92 C   |
| T142A+ N327S+ K425E+ K520R+ N595I |        |        |        | 93 C   |
| F188L + D261G + T288P             | 75 C   |        | 95 C   |        |

The results show improved thermostability for each variant. One variant shows an improvement of more than 10 C at pH 4.0 and 5.5.

#### 5 Example 4: Specific activity of variants

Amylase activity was determined by a colorimetric measurement after action on Phadebas tablets at pH 5.0 and 60°C. The results for two Novamyl variants, relative to Novamyl were as follows:

| Modifications | Relative amylase activity |
|---------------|---------------------------|
| None (parent) | 100                       |
| 192-A-193     | 110                       |
| Δ (191-195)   | 300                       |

10

The specific activity was further tested by action on maltotriose at pH 4.0, 60°C by the MANU method described above. The results showed that the variant G370N, N371G has a maltotriose activity of 106 % compared to Novamyl.

#### Example 5: Inhibition of retrogradation

15 The efficiency of Novamyl and Novamyl variants to inhibit retrogradation was determined as follows:

730 mg of 50 % (w/w) amylopectin slurry in 0.1 M sodium acetate, at a selected pH (3.7, 4.3 or 5.5) was mixed with 20 µl of an enzyme sample, and the mixture was incubated in a sealed ampoule for 1 hour at 40°C, followed by incubation at 100 °C for  
20 1 hour in order to gelatinize the samples. The sample was then aged for 7 days at room temperature to allow recrystallization of the amylopectin. A control without enzyme was included.

After aging, DSC was performed on the sample by scanning from 5°C to 95°C at a constant scan rate of 90°C/hour. The area under the first endothermic peak in the  
25 thermogram was taken to represent the amount of retrograded amylopectin, and the



relative inhibition of retrogradation was taken as the area reduction (in %) relative to the control without enzyme.

In the table below, the efficiency of the enzyme is expressed as the ratio of the relative inhibition of retrogradation to the enzyme dosage (in MANU/ml):

5

| pH  | Modifications                     | MANU/ml | Relative inhibition | Efficiency |
|-----|-----------------------------------|---------|---------------------|------------|
| 3.7 | A30D+ K40R+ D261G                 | 0.23    | 0.38                | 1.7        |
| 3.7 | T142A+ N327S+ K425E+ K520R+ N595I | 0.07    | 0.29                | 4.1        |
| 3.7 | None (parent)                     | 0.27    | 0.38                | 1.4        |
| 4.3 | N115D+ F188L                      | 0.01    | 0.18                | 18         |
| 4.3 | None (parent)                     | 0.27    | 0.43                | 1.6        |
| 5.5 | Δ (191-195)+ F188L+ T189Y         | 0.02    | 0.12                | 6          |
| 5.5 | Δ (191-195)                       | 0.02    | 0.14                | 7          |
| 5.5 | Δ (191-195)                       | 0.05    | 0.31                | 6.2        |
| 5.5 | N115D+ F188L                      | 0.01    | 0.39                | 39         |
| 5.5 | T142A+ D261G                      | 0.14    | 0.53                | 3.8        |
| 5.5 | None (parent)                     | 0.27    | 0.49                | 1.8        |

The results demonstrate that a number of variants are more efficient than the parent amylase to inhibit retrogradation.

#### Example 6: Anti-staling effect of variants

10 Bread was made by an European Straight Dough method (wheat flour, water, yeast, salt, sugar, ascorbic acid) or from a wheat sour dough (acidified with "Ireks ferdigsauer" from Balchem Co.) with or without addition of enzymes, and loaves were baked in lidded pans, to avoid volume effects. pH in the dough was measured by blending 10 g of the mixed dough with 100 ml of deionised water for 30 min before  
15 measurement of pH in the suspension. The bread was allowed to cool for 2 hours, and the texture was analyzed by a Texture Analyser TA-XT2 from Stable Micro Systems. The remaining loaves were then wrapped in plastic bags and stored at room temperature for texture analysis after 1, 4 and 7 days.

The texture analysis of each loaf was done by cutting 4 slices; the force was  
20 measured at 25 % compression (P1), at 40% compression (P2) and after keeping 40%

compression constant for 30 sec. (P3). P1 was taken as the firmness (in grams), and the ratio (P3/P2) was taken as the elasticity of the crumb. The extent of retrogradation after 7 days storage was determined by DSC as described in Example 7.

European Straight Dough (pH5.5-6.0)

- 5 A Novamyl variant (T142A+ N327S+ K425E+ K520R+ N595I) was tested at dosages in the range of 0-2 mg enzyme/kg flour, and the parent enzyme (Novamyl) was used for comparison.

The following results were obtained for elasticity (P3/P2) after two hours and 7 days and firmness (P1) after 7 days:

10

| Enzyme  | Dosage<br>mg/kg flour | Elasticity<br>2 hours | Elasticity<br>1 day | Elasticity<br>7 days |
|---------|-----------------------|-----------------------|---------------------|----------------------|
| None    | 0                     | 0.69                  | 0.60                | 0.44                 |
| Parent  | 1                     | 0.62                  | 0.60                | 0.55                 |
|         | 2                     | 0.58                  | 0.57                | 0.54                 |
| Variant | 1                     | 0.65                  | 0.62                | 0.56                 |
|         | 2                     | 0.63                  | 0.61                | 0.58                 |

| Enzyme  | Dosage<br>mg/kg flour | Firmness (P1)<br>after 7 days |
|---------|-----------------------|-------------------------------|
| None    | 0                     | 2267                          |
| Parent  | 1                     | 1192                          |
|         | 2                     | 1113                          |
| Variant | 1                     | 1022                          |
|         | 2                     | 905                           |

- 15 The results after two hours and 1 day show that at equal dosages, the variant gives a better elasticity than the parent enzyme. The results after 7 days show that the variant at dosages of 1-2 mg/kg gives a softer crumb (lower firmness and higher elasticity) than the parent enzyme at the same dosage. Thus, the variant has a better anti-staling effect throughout a 7-day storage period.

Sour dough (pH approx. 4.5)

A Novamyl variant (F188L+ D261G+ T288P) was tested in sour dough, and the parent enzyme (Novamyl) was used for comparison. The following results were obtained for firmness (P1) after 7 days, elasticity (P3/P2) after 4 and 7 days and retrogradation after 7 days:

| Enzyme  | Dosage<br>mg/kg flour | Firmness (P1)<br>after 7 days |
|---------|-----------------------|-------------------------------|
| None    | 0                     | 2590                          |
| Parent  | 1                     | 2031                          |
|         | 3                     | 1912                          |
|         | 13                    | 1570                          |
| Variant | 1                     | 1436                          |
|         | 3                     | 1226                          |

| Enzyme  | Dosage<br>mg/kg flour | Elasticity<br>4 days | Elasticity<br>7 days |
|---------|-----------------------|----------------------|----------------------|
| None    | 0                     | 0.49                 | 0.47                 |
| Parent  | 1                     | 0.51                 | 0.52                 |
|         | 3                     | 0.53                 | 0.51                 |
|         | 13                    | 0.53                 | 0.51                 |
| Variant | 1                     | 0.59                 | 0.57                 |
|         | 3                     | 0.57                 | 0.58                 |

| Enzyme  | Dosage<br>mg/kg flour | Retrogradation, 7 days<br>(relative to control) |
|---------|-----------------------|---|
| None    | 0                     | 100 %   |
| Parent  | 1                     | 100 %   |
|         | 3                     | 63 %  |
|         | 13                    | 32 %  |
| Variant | 1                     | 46 %  |
|         | 3                     | 20 %  |

The results show that the variant has a markedly improved effect on texture evaluated as firmness and elasticity in sour dough at pH 4.5. A dosage of 1-3 mg/kg of the variant is superior to 13 mg/kg of the parent enzyme on all parameters tested, and the elasticity achieved with the variant cannot be matched by the parent enzyme at any dosage.

pH-profile in wheat-flour bread (pH approx. 4.4; 4.9; and 5.5)

The Novamyl variant (F188L+ D261G+ T288P) was further tested in acidified wheat flour bread to measure the function over a broader pH range in baking application, while maintaining a comparable recipe. The parent enzyme (Novamyl) was used for comparison. Dosage of the parent enzyme was changed at the various pH to compensate for the lower activity of the parent enzyme at lower pH. The following results were obtained for firmness (P1) and elasticity (P3/P2) after 0 (= 2 hours), 1, 3 and 7 days.

15

| pH     | Enzyme  | Dosage<br>mg/kg<br>flour | Firmness |       |        |        |
|--------|---------|--------------------------|----------|-------|--------|--------|
|        |         |                          | 0 days   | 1 day | 3 days | 7 days |
| pH 4.4 | None    | 0                        | 450      | 1144  | 1945   | 3020   |
|        | Variant | 0.5                      | 392      | 939   | 1386   | 1664   |
|        | Parent  | 15                       | 870      | 1206  | 1220   | 1511   |
|        | Parent  | 1                        | 586      | 1127  | 2005   | 2312   |
| pH 4.9 | None    | 0                        | 330      | 764   | 1536   | 2005   |
|        | Variant | 0.5                      | 287      | 687   | 767    | 1096   |
|        | Parent  | 7                        | 570      | 1075  | 984    | 1057   |
|        | Parent  | 0.5                      | 373      | 784   | 1170   | 1642   |
| pH 5.5 | None    | 0                        | 217      | 711   | 1123   | 1382   |
|        | Variant | 0.5                      | 315      | 447   | 712    | 846    |
|        | Parent  | 3.5                      | 431      | 629   | 666    | 718    |
|        | Parent  | 0.5                      | 381      | 599   | 630    | 922    |

| pH     | Enzyme  | Dosage<br>mg/kg<br>flour | Elasticity |       |        |        |
|--------|---------|--------------------------|------------|-------|--------|--------|
|        |         |                          | 0 days     | 1 day | 3 days | 7 days |
| pH 4.4 | None    | 0                        | 0.70       | 0.61  | 0.53   | 0.48   |
|        | Variant | 0.5                      | 0.70       | 0.63  | 0.59   | 0.56   |
|        | Parent  | 15                       | 0.53       | 0.50  | 0.52   | 0.51   |
|        | Parent  | 1                        | 0.65       | 0.60  | 0.55   | 0.51   |
| pH 4.9 | None    | 0                        | 0.71       | 0.64  | 0.55   | 0.49   |
|        | Variant | 0.5                      | 0.70       | 0.65  | 0.63   | 0.60   |
|        | Parent  | 7                        | 0.56       | 0.52  | 0.54   | 0.54   |
|        | Parent  | 0.5                      | 0.67       | 0.61  | 0.58   | 0.54   |
| pH 5.5 | None    | 0                        | 0.70       | 0.61  | 0.56   | 0.51   |
|        | Variant | 0.5                      | 0.68       | 0.64  | 0.61   | 0.60   |
|        | Parent  | 3.5                      | 0.58       | 0.56  | 0.57   | 0.57   |
|        | Parent  | 0.5                      | 0.63       | 0.61  | 0.62   | 0.58   |

It is clearly observed, that the variant is much improved compared to the parent at all pH, and especially at lower pH. The elasticity is higher, and the crumb stays more soft over the measured time span.

#### Four variants tested in wheat sourdough compared to parent enzyme

Four Novamyl variants were tested in another test series of acidified wheat flour bread to determine the performance in sourdough baking application. pH in the bread and dough was measured to be in the interval 4.30-4.40. The parent enzyme (Novamyl) was used for comparison. Dosage of the parent enzyme was chosen at 1 and 13 mg/kg flour, much higher than the variants, as we have experienced that this is needed to see effect of the parent enzyme in this specific application. The firmness (P1) and elasticity (P3/P2) were determined after 1, 3 and 7 days, and the extent of retrogradation after 7 days storage was determined as described above.

| Enzyme                                     | Dosage<br>mg/kg flour | Firmness |        |        |
|--|-----------------------|----------|--------|--------|
|  |                       | 1 day    | 3 days | 7 days |
| None                                       | 0                     | 789      | 1624   | 2054   |
| Parent                                     | 1                     | 745      | 1107   | 1685   |
|  | 13                    | 722      | 967    | 1205   |
| N26S +F188L +D261G +T288P<br>+T594A +I600V | 0,5                   | 716      | 1170   | 1518   |
|  | 3                     | 847      | 895    | 1188   |
| F188L +D261G +T288P                        | 0.5                   | 689      | 1054   | 1457   |
| A197P +D261G +T288P +N342S                 | 0.5                   | 638      | 1114   | 1631   |
| F188L +D261G +T288P +A483T                 | 0.5                   | 643      | 983    | 1562   |
|  | 3                     | 660      | 804    | 953    |

| Enzyme                                     | Dosage<br>mg/kg flour | Elasticity |        |        |
|--|-----------------------|------------|--------|--------|
|  |                       | 1 day      | 3 days | 7 days |
| None                                       | 0                     | 0.63       | 0.55   | 0.48   |
| Parent                                     | 1                     | 0.64       | 0.57   | 0.49   |
|  | 13                    | 0.57       | 0.56   | 0.53   |
| N26S +F188L +D261G +T288P<br>+T594A +I600V | 0.5                   | 0.63       | 0.56   | 0.50   |
|  | 3                     | 0.61       | 0.59   | 0.57   |
| F188L +D261G +T288P                        | 0.5                   | 0.64       | 0.58   | 0.53   |
| A197P +D261G +T288P +N342S                 | 0.5                   | 0.64       | 0.57   | 0.50   |
| F188L +D261G +T288P +A483T                 | 0.5                   | 0.65       | 0.58   | 0.53   |
|  | 3                     | 0.63       | 0.60   | 0.58   |

| Enzyme                                     | Dosage<br>mg/kg flour | Retrogradation, 7<br>days<br>(relative to control) |
|--|-----------------------|--|
| None                                       | 0                     | 100 %  |
| Parent                                     | 1<br>13               | 67 %<br>21 %                                       |
| N26S +F188L +D261G +T288P<br>+T594A +I600V | 0.5<br>3              | 72 %<br>18 %                                       |
| F188L +D261G +T288P                        | 0.5                   | 53 %   |
| A197P +D261G +T288P +N342S                 | 0.5                   | 59 %   |
| F188L +D261G +T288P +A483T                 | 0.5<br>3              | 43 %<br>10 %                                       |

For antistaling (fresh-keeping) it is particularly important, that the bread is soft and elastic after several days storage. Therefore, most weight should be put on the textural properties after 7 days of storage. It is clearly observed, that the variants are much improved compared to the parent. The elasticity is higher, and the crumb stays more soft.

#### Example 7: Cleavage pattern of variants

The cleavage pattern in starch hydrolysis was compared for two variants and the parent enzyme, Novamyl.

The results below indicate % by weight of each oligosaccharide (G1-G8) formed after 24 hours incubation in 1% (w/v) starch using 50 mM sodium acetate, 1 mM CaCl<sub>2</sub>, pH 5.0 at 50 °C. The oligosaccharides were identified and quantitated using HPLC.

| Oligosaccharide | Parent | $\Delta$ (191-195) | N115D+ F188L |
|-----------------|--------|--------------------|--------------|
| G8              | -      | 1.7                | -            |
| G7              | -      | 2.6                | -            |
| G6              | -      | 7.5                | 1.4          |

|           |      |      |      |
|-----------|------|------|------|
| <b>G5</b> | -    | 10.1 | 2.1  |
| <b>G4</b> | -    | 21.1 | 11.3 |
| <b>G3</b> | -    | 28.7 | 10.7 |
| <b>G2</b> | 96.5 | 28.3 | 61.9 |
| <b>G1</b> | 3.5  | -    | 12.6 |

The results demonstrate a significantly altered cleavage pattern. Novamyl after 24 hours produces mainly maltose and virtually no higher oligosaccharides. In contrast, the two variants produce significant amounts of maltotriose and higher oligosaccharides.

#### **Example 8: Substrate specificity of variants**

The activity of variants was tested on two different substrates: glucose release from maltotriose and color release from Phadebas colored starch. The parent enzyme (Novamyl) was tested for comparison. The measurements were made at pH 5, and each activity was expressed relative to the parent enzyme. The ratio of activities on the two substrates was found to be as follows:

| <b>Variant</b>                                 | <b>Activity ratio<br/>Starch/maltotriose</b> |
|--|--|
| <b>Parent enzyme</b>                           | 1.0  |
| <b>F188L, D261G, T288P</b>                     | 3.6  |
| <b>N26S +F188L, D261G, T288P, T594A, I600V</b> | 5.5  |
| <b>N26S, T80A, F188L, D261G, T288P, R291L</b>  | 1.9  |
| <b>A197P, D261G, T288P, N342S</b>              | 1.5  |
| <b>T142A, D261G, T288P, Q449R</b>              | 2.5  |
| <b>F188L, D261G, T288P, A483T</b>              | 2.5  |

It is seen that the 6 variants have an increased activity on starch relative to maltotriose.

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|    |     |     |   |   |        |        |        |      |       |   |     |     |     |   |    |        |        |        |      |       |   |
|----|-----|-----|---|---|--------|--------|--------|------|-------|---|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 1  | N   | SER | A | 1 | 10.254 | 56.595 | 38.175 | 1.00 | 15.64 | 7 | 43  | CD  | LYS | A | 7  | 18.160 | 63.123 | 46.350 | 1.00 | 9.80  | 6 |
| 2  | CA  | SER | A | 1 | 11.216 | 55.462 | 37.898 | 1.00 | 15.87 | 6 | 44  | CE  | LYS | A | 7  | 17.698 | 64.488 | 45.795 | 1.00 | 10.87 | 6 |
| 3  | C   | SER | A | 1 | 12.466 | 55.723 | 38.726 | 1.00 | 14.53 | 6 | 45  | NZ  | LYS | A | 7  | 17.114 | 64.187 | 44.425 | 1.00 | 11.38 | 7 |
| 4  | O   | SER | A | 1 | 12.585 | 56.773 | 39.369 | 1.00 | 15.99 | 8 | 46  | N   | GLY | A | 8  | 21.036 | 58.214 | 45.577 | 1.00 | 13.10 | 7 |
| 5  | CB  | SER | A | 1 | 11.527 | 55.345 | 36.397 | 1.00 | 21.54 | 6 | 47  | CA  | GLY | A | 8  | 21.604 | 56.982 | 46.166 | 1.00 | 12.31 | 6 |
| 6  | OG  | SER | A | 1 | 12.305 | 56.503 | 36.045 | 1.00 | 20.33 | 8 | 48  | C   | GLY | A | 8  | 22.718 | 56.358 | 45.340 | 1.00 | 14.02 | 6 |
| 7  | N   | SER | A | 2 | 13.466 | 54.795 | 38.551 | 1.00 | 18.07 | 7 | 49  | O   | GLY | A | 8  | 23.109 | 55.205 | 45.579 | 1.00 | 13.36 | 8 |
| 8  | CA  | SER | A | 2 | 14.705 | 55.061 | 39.291 | 1.00 | 19.33 | 6 | 50  | N   | ASP | A | 9  | 23.133 | 57.048 | 44.293 | 1.00 | 11.90 | 7 |
| 9  | C   | SER | A | 2 | 15.621 | 56.069 | 38.559 | 1.00 | 15.87 | 6 | 51  | CA  | ASP | A | 9  | 24.049 | 56.447 | 43.319 | 1.00 | 11.74 | 6 |
| 10 | O   | SER | A | 2 | 16.573 | 56.563 | 39.209 | 1.00 | 16.73 | 8 | 52  | C   | ASP | A | 9  | 25.478 | 56.996 | 43.442 | 1.00 | 10.18 | 6 |
| 11 | CB  | SER | A | 2 | 15.490 | 53.735 | 39.422 | 1.00 | 26.53 | 6 | 106 | CB  | ILE | A | 15 | 37.192 | 59.653 | 28.343 | 1.00 | 10.73 | 6 |
| 12 | OG  | SER | A | 2 | 15.918 | 53.392 | 38.123 | 1.00 | 21.07 | 8 | 107 | CG1 | ILE | A | 15 | 37.106 | 60.975 | 29.131 | 1.00 | 11.86 | 6 |
| 13 | N   | SER | A | 3 | 15.136 | 56.545 | 37.384 | 1.00 | 12.71 | 7 | 108 | CG2 | ILE | A | 15 | 37.626 | 60.014 | 26.904 | 1.00 | 12.56 | 6 |
| 14 | CA  | SER | A | 3 | 15.956 | 57.522 | 36.680 | 1.00 | 13.38 | 6 | 109 | CD1 | ILE | A | 15 | 36.181 | 62.091 | 28.574 | 1.00 | 15.42 | 6 |
| 15 | C   | SER | A | 3 | 15.873 | 58.916 | 37.316 | 1.00 | 12.57 | 6 | 110 | N   | ILE | A | 16 | 34.926 | 57.450 | 26.561 | 1.00 | 10.37 | 7 |
| 16 | O   | SER | A | 3 | 16.759 | 59.749 | 37.029 | 1.00 | 15.22 | 8 | 111 | CA  | ILE | A | 16 | 34.728 | 56.178 | 25.868 | 1.00 | 11.03 | 6 |
| 17 | CB  | SER | A | 3 | 15.434 | 57.682 | 35.219 | 1.00 | 16.30 | 6 | 112 | C   | ILE | A | 16 | 35.990 | 55.729 | 25.099 | 1.00 | 12.23 | 6 |
| 18 | OG  | SER | A | 3 | 15.593 | 56.381 | 34.568 | 1.00 | 23.61 | 8 | 113 | O   | ILE | A | 16 | 36.342 | 54.511 | 25.184 | 1.00 | 11.07 | 8 |
| 19 | N   | ALA | A | 4 | 14.811 | 59.222 | 38.050 | 1.00 | 10.88 | 7 | 114 | CB  | ILE | A | 16 | 33.578 | 56.292 | 24.863 | 1.00 | 10.56 | 6 |
| 20 | CA  | ALA | A | 4 | 14.574 | 60.623 | 38.384 | 1.00 | 11.38 | 6 | 115 | CG1 | ILE | A | 16 | 32.240 | 56.387 | 25.709 | 1.00 | 11.92 | 6 |
| 21 | C   | ALA | A | 4 | 15.599 | 61.115 | 39.409 | 1.00 | 12.81 | 6 | 116 | CG2 | ILE | A | 16 | 33.444 | 55.053 | 23.953 | 1.00 | 11.18 | 6 |
| 22 | O   | ALA | A | 4 | 15.888 | 62.314 | 39.355 | 1.00 | 12.58 | 8 | 117 | CD1 | ILE | A | 16 | 31.115 | 56.958 | 24.823 | 1.00 | 13.67 | 6 |
| 23 | CB  | ALA | A | 4 | 13.132 | 60.682 | 38.956 | 1.00 | 14.28 | 6 | 118 | N   | ASP | A | 17 | 36.565 | 56.624 | 24.314 | 1.00 | 10.08 | 7 |
| 24 | N   | SER | A | 5 | 15.968 | 60.306 | 40.380 | 1.00 | 13.21 | 7 | 119 | CA  | ASP | A | 17 | 37.730 | 56.165 | 23.518 | 1.00 | 8.61  | 6 |
| 25 | CA  | SER | A | 5 | 16.905 | 60.780 | 41.427 | 1.00 | 14.29 | 6 | 120 | C   | ASP | A | 17 | 38.911 | 55.693 | 24.346 | 1.00 | 10.86 | 6 |
| 26 | C   | SER | A | 5 | 18.163 | 59.941 | 41.357 | 1.00 | 16.01 | 6 | 121 | O   | ASP | A | 17 | 39.777 | 54.987 | 23.831 | 1.00 | 11.03 | 8 |
| 27 | O   | SER | A | 5 | 18.053 | 58.724 | 41.237 | 1.00 | 16.41 | 8 | 122 | CB  | ASP | A | 17 | 38.184 | 57.422 | 22.675 | 1.00 | 11.30 | 6 |
| 28 | CB  | SER | A | 5 | 16.218 | 60.613 | 42.785 | 1.00 | 15.57 | 6 | 123 | CG  | ASP | A | 17 | 39.380 | 57.017 | 21.755 | 1.00 | 9.77  | 6 |
| 29 | OG  | SER | A | 5 | 17.193 | 60.855 | 43.843 | 1.00 | 13.17 | 8 | 124 | OD1 | ASP | A | 17 | 39.105 | 56.206 | 20.852 | 1.00 | 11.65 | 8 |
| 30 | N   | VAL | A | 6 | 19.340 | 60.530 | 41.476 | 1.00 | 10.07 | 7 | 125 | OD2 | ASP | A | 17 | 40.480 | 57.562 | 21.970 | 1.00 | 11.48 | 8 |
| 31 | CA  | VAL | A | 6 | 20.589 | 59.751 | 41.567 | 1.00 | 10.13 | 6 | 126 | N   | ARG | A | 18 | 38.972 | 55.999 | 25.646 | 1.00 | 9.54  | 7 |
| 32 | C   | VAL | A | 6 | 21.169 | 59.955 | 42.963 | 1.00 | 10.99 | 6 | 127 | CA  | ARG | A | 18 | 40.113 | 55.719 | 26.527 | 1.00 | 8.38  | 6 |
| 33 | O   | VAL | A | 6 | 22.349 | 59.685 | 43.172 | 1.00 | 10.81 | 8 | 128 | C   | ARG | A | 18 | 39.826 | 54.720 | 27.608 | 1.00 | 9.97  | 6 |
| 34 | CB  | VAL | A | 6 | 21.639 | 60.160 | 40.513 | 1.00 | 13.85 | 6 | 129 | O   | ARG | A | 18 | 40.643 | 54.490 | 28.501 | 1.00 | 13.32 | 8 |
| 35 | CG1 | VAL | A | 6 | 21.002 | 59.694 | 39.148 | 1.00 | 15.29 | 6 | 130 | CB  | ARG | A | 18 | 40.537 | 57.083 | 27.137 | 1.00 | 11.02 | 6 |
| 36 | CG2 | VAL | A | 6 | 21.874 | 61.656 | 40.459 | 1.00 | 12.12 | 6 | 131 | CG  | ARG | A | 18 | 40.931 | 58.139 | 26.063 | 1.00 | 9.63  | 6 |
| 37 | N   | LYS | A | 7 | 20.369 | 60.349 | 43.964 | 1.00 | 10.30 | 7 | 132 | CD  | ARG | A | 18 | 42.135 | 57.721 | 25.237 | 1.00 | 9.86  | 6 |
| 38 | CA  | LYS | A | 7 | 20.901 | 60.604 | 45.331 | 1.00 | 9.78  | 6 | 133 | NE  | ARG | A | 18 | 42.280 | 58.523 | 23.969 | 1.00 | 10.16 | 7 |
| 39 | C   | LYS | A | 7 | 21.508 | 59.360 | 46.015 | 1.00 | 12.06 | 6 | 134 | CZ  | ARG | A | 18 | 43.103 | 59.578 | 23.903 | 1.00 | 13.46 | 6 |
| 40 | O   | LYS | A | 7 | 22.382 | 59.560 | 46.857 | 1.00 | 12.59 | 8 | 135 | NH1 | ARG | A | 18 | 43.748 | 60.063 | 24.966 | 1.00 | 12.03 | 7 |
| 41 | CB  | LYS | A | 7 | 19.830 | 61.187 | 46.264 | 1.00 | 11.40 | 6 | 136 | NH2 | ARG | A | 18 | 43.350 | 60.181 | 22.725 | 1.00 | 10.43 | 7 |
| 42 | CG  | LYS | A | 7 | 19.414 | 62.588 | 45.680 | 1.00 | 12.09 | 6 | 137 | N   | PHE | A | 19 | 38.648 | 54.007 | 27.497 | 1.00 | 11.25 | 7 |



|     |     |       |    |        |        |        |      |       |   |     |     |       |    |        |        |        |      |       |   |
|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| 222 | CB  | PRO A | 29 | 35.087 | 53.483 | 10.312 | 1.00 | 17.71 | 6 | 264 | O   | LEU A | 35 | 42.472 | 58.755 | 15.182 | 1.00 | 14.18 | 8 |
| 223 | CG  | PRO A | 29 | 35.394 | 53.615 | 11.787 | 1.00 | 17.95 | 6 | 265 | CB  | LEU A | 35 | 40.784 | 59.737 | 13.090 | 1.00 | 10.53 | 6 |
| 224 | CD  | PRO A | 29 | 36.907 | 53.841 | 11.957 | 1.00 | 15.54 | 6 | 266 | CG  | LEU A | 35 | 40.170 | 60.460 | 11.891 | 1.00 | 12.89 | 6 |
| 225 | N   | ALA A | 30 | 36.329 | 53.244 | 7.331  | 1.00 | 16.99 | 7 | 267 | CD1 | LEU A | 35 | 38.783 | 61.033 | 12.240 | 1.00 | 13.47 | 6 |
| 226 | CA  | ALA A | 30 | 36.533 | 54.024 | 6.117  | 1.00 | 19.06 | 6 | 268 | CD2 | LEU A | 35 | 41.090 | 61.613 | 11.433 | 1.00 | 15.36 | 6 |
| 227 | C   | ALA A | 30 | 35.841 | 55.375 | 6.161  | 1.00 | 16.15 | 6 | 269 | N   | TYR A | 36 | 43.025 | 57.036 | 13.757 | 1.00 | 13.30 | 7 |
| 228 | O   | ALA A | 30 | 36.398 | 56.355 | 5.599  | 1.00 | 18.27 | 8 | 270 | CA  | TYR A | 36 | 43.335 | 56.061 | 14.796 | 1.00 | 13.00 | 6 |
| 229 | CB  | ALA A | 30 | 35.998 | 53.268 | 4.880  | 1.00 | 21.27 | 6 | 271 | C   | TYR A | 36 | 44.826 | 55.913 | 15.032 | 1.00 | 15.18 | 6 |
| 230 | N   | LYS A | 31 | 34.697 | 55.514 | 6.833  | 1.00 | 15.01 | 7 | 272 | O   | TYR A | 36 | 45.610 | 55.855 | 14.049 | 1.00 | 15.86 | 8 |
| 231 | CA  | LYS A | 31 | 34.012 | 56.812 | 6.886  | 1.00 | 14.64 | 6 | 273 | CB  | TYR A | 36 | 42.749 | 54.728 | 14.291 | 1.00 | 13.61 | 6 |
| 232 | C   | LYS A | 31 | 34.944 | 57.908 | 7.416  | 1.00 | 15.07 | 6 | 274 | CG  | TYR A | 36 | 43.149 | 53.492 | 15.076 | 1.00 | 12.30 | 6 |
| 233 | O   | LYS A | 31 | 34.722 | 59.094 | 7.172  | 1.00 | 14.25 | 8 | 275 | CD1 | TYR A | 36 | 42.927 | 53.383 | 16.454 | 1.00 | 14.21 | 6 |
| 234 | CB  | LYS A | 31 | 32.771 | 56.667 | 7.818  | 1.00 | 13.99 | 6 | 276 | CD2 | TYR A | 36 | 43.807 | 52.460 | 14.391 | 1.00 | 16.88 | 6 |
| 235 | CG  | LYS A | 31 | 31.981 | 57.980 | 8.050  | 1.00 | 13.23 | 6 | 277 | CE1 | TYR A | 36 | 43.317 | 52.206 | 17.122 | 1.00 | 14.97 | 6 |
| 236 | CD  | LYS A | 31 | 30.617 | 57.569 | 8.669  | 1.00 | 16.17 | 6 | 278 | CE2 | TYR A | 36 | 44.182 | 51.320 | 15.075 | 1.00 | 19.02 | 6 |
| 237 | CE  | LYS A | 31 | 29.763 | 58.766 | 9.053  | 1.00 | 14.65 | 6 | 279 | CZ  | TYR A | 36 | 43.930 | 51.206 | 16.416 | 1.00 | 17.90 | 6 |
| 238 | NZ  | LYS A | 31 | 30.427 | 59.568 | 10.156 | 1.00 | 12.05 | 7 | 280 | OH  | TYR A | 36 | 44.299 | 50.063 | 17.135 | 1.00 | 18.88 | 8 |
| 239 | N   | SER A | 32 | 35.822 | 57.610 | 8.364  | 1.00 | 16.27 | 7 | 281 | N   | ASP A | 37 | 45.211 | 55.848 | 16.289 | 1.00 | 12.45 | 7 |
| 240 | CA  | SER A | 32 | 36.675 | 58.587 | 9.038  | 1.00 | 14.39 | 6 | 282 | CA  | ASP A | 37 | 46.646 | 55.624 | 16.621 | 1.00 | 12.80 | 6 |
| 241 | C   | SER A | 32 | 38.087 | 57.989 | 9.161  | 1.00 | 17.62 | 6 | 283 | C   | ASP A | 37 | 46.700 | 54.350 | 17.441 | 1.00 | 14.03 | 6 |
| 242 | O   | SER A | 32 | 38.770 | 57.968 | 10.193 | 1.00 | 17.19 | 8 | 284 | O   | ASP A | 37 | 46.507 | 54.281 | 18.673 | 1.00 | 13.32 | 8 |
| 243 | CB  | SER A | 32 | 36.100 | 58.851 | 10.460 | 1.00 | 12.32 | 6 | 285 | CB  | ASP A | 37 | 47.120 | 56.834 | 17.463 | 1.00 | 13.46 | 6 |
| 244 | OG  | SER A | 32 | 35.874 | 57.664 | 11.167 | 1.00 | 12.92 | 8 | 286 | CG  | ASP A | 37 | 48.543 | 56.543 | 17.991 | 1.00 | 20.57 | 6 |
| 245 | N   | TYR A | 33 | 38.596 | 57.524 | 8.010  | 1.00 | 14.71 | 7 | 287 | OD1 | ASP A | 37 | 49.278 | 55.720 | 17.366 | 1.00 | 17.00 | 8 |
| 246 | CA  | TYR A | 33 | 39.875 | 56.801 | 8.045  | 1.00 | 15.23 | 6 | 288 | OD2 | ASP A | 37 | 48.902 | 57.113 | 19.028 | 1.00 | 17.32 | 8 |
| 247 | C   | TYR A | 33 | 41.051 | 57.676 | 8.444  | 1.00 | 14.94 | 6 | 289 | N   | PRO A | 38 | 47.163 | 53.245 | 16.821 | 1.00 | 15.62 | 7 |
| 248 | O   | TYR A | 33 | 41.042 | 58.848 | 8.023  | 1.00 | 17.62 | 8 | 290 | CA  | PRO A | 38 | 47.375 | 52.024 | 17.548 | 1.00 | 15.67 | 6 |
| 249 | CB  | TYR A | 33 | 40.075 | 56.295 | 6.582  | 1.00 | 18.09 | 6 | 291 | C   | PRO A | 38 | 48.484 | 52.056 | 18.558 | 1.00 | 15.69 | 6 |
| 250 | CG  | TYR A | 33 | 41.166 | 55.254 | 6.536  | 1.00 | 20.46 | 6 | 292 | O   | PRO A | 38 | 48.513 | 51.189 | 19.436 | 1.00 | 18.95 | 8 |
| 251 | CD1 | TYR A | 33 | 40.982 | 53.978 | 7.004  | 1.00 | 26.95 | 6 | 293 | CB  | PRO A | 38 | 47.669 | 50.946 | 16.450 | 1.00 | 17.01 | 6 |
| 252 | CD2 | TYR A | 33 | 42.408 | 55.618 | 6.002  | 1.00 | 31.14 | 6 | 294 | CG  | PRO A | 38 | 48.367 | 51.843 | 15.437 | 1.00 | 18.68 | 6 |
| 253 | CE1 | TYR A | 33 | 41.994 | 53.027 | 6.944  | 1.00 | 33.56 | 6 | 295 | CD  | PRO A | 38 | 47.570 | 53.192 | 15.409 | 1.00 | 18.22 | 6 |
| 254 | CE2 | TYR A | 33 | 43.422 | 54.670 | 5.943  | 1.00 | 31.30 | 6 | 296 | N   | THR A | 39 | 49.385 | 53.031 | 18.514 | 1.00 | 15.60 | 7 |
| 255 | CZ  | TYR A | 33 | 43.210 | 53.409 | 6.402  | 1.00 | 33.88 | 6 | 297 | CA  | THR A | 39 | 50.469 | 53.080 | 19.499 | 1.00 | 14.85 | 6 |
| 256 | OH  | TYR A | 33 | 44.235 | 52.483 | 6.334  | 1.00 | 44.90 | 8 | 298 | C   | THR A | 39 | 50.126 | 53.773 | 20.822 | 1.00 | 17.68 | 6 |
| 257 | N   | GLY A | 34 | 42.039 | 57.105 | 9.114  | 1.00 | 12.92 | 7 | 299 | O   | THR A | 39 | 50.961 | 53.777 | 21.719 | 1.00 | 17.01 | 8 |
| 258 | CA  | GLY A | 34 | 43.281 | 57.836 | 9.403  | 1.00 | 14.92 | 6 | 300 | CB  | THR A | 39 | 51.692 | 53.847 | 18.947 | 1.00 | 19.14 | 6 |
| 259 | C   | GLY A | 34 | 43.255 | 58.672 | 10.686 | 1.00 | 15.08 | 6 | 301 | OG1 | THR A | 39 | 51.503 | 55.239 | 18.723 | 1.00 | 16.66 | 8 |
| 260 | O   | GLY A | 34 | 44.274 | 59.342 | 10.956 | 1.00 | 15.24 | 8 | 302 | CG2 | THR A | 39 | 52.083 | 53.233 | 17.573 | 1.00 | 22.20 | 6 |
| 261 | N   | LEU A | 35 | 42.253 | 58.417 | 11.548 | 1.00 | 12.52 | 7 | 303 | N   | LYS A | 40 | 48.983 | 54.487 | 20.832 | 1.00 | 14.93 | 7 |
| 262 | CA  | LEU A | 35 | 42.215 | 59.140 | 12.846 | 1.00 | 11.02 | 6 | 304 | CA  | LYS A | 40 | 48.588 | 55.225 | 22.041 | 1.00 | 14.22 | 6 |
| 263 | C   | LEU A | 35 | 42.519 | 58.271 | 14.028 | 1.00 | 15.01 | 6 | 305 | C   | LYS A | 40 | 49.736 | 56.141 | 22.483 | 1.00 | 17.80 | 6 |

|     |     |       |    |        |        |        |      |       |   |     |     |        |    |        |        |        |      |       |    |
|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|--------|----|--------|--------|--------|------|-------|----|
| 306 | O   | LYS A | 40 | 50.009 | 56.348 | 23.685 | 1.00 | 17.78 | 8 | 348 | CE  | LYS A  | 44 | 45.254 | 68.171 | 22.334 | 1.00 | 15.83 | 6  |
| 307 | CB  | LYS A | 40 | 48.104 | 54.324 | 23.207 | 1.00 | 19.03 | 6 | 349 | NZ  | LYS A  | 44 | 45.125 | 69.681 | 22.068 | 1.00 | 18.92 | 7  |
| 308 | CG  | LYS A | 40 | 47.023 | 53.320 | 22.775 | 1.00 | 18.65 | 6 | 350 | N   | MET A  | 45 | 44.473 | 61.576 | 19.114 | 1.00 | 10.42 | 7  |
| 309 | CD  | LYS A | 40 | 46.535 | 52.543 | 24.031 | 1.00 | 21.38 | 6 | 351 | CA  | MET A  | 45 | 43.881 | 60.686 | 18.112 | 1.00 | 12.24 | 6  |
| 310 | CE  | LYS A | 40 | 45.432 | 51.573 | 23.590 | 1.00 | 22.34 | 6 | 352 | C   | MET A  | 45 | 42.952 | 59.664 | 18.768 | 1.00 | 11.36 | 6  |
| 311 | NZ  | LYS A | 40 | 45.883 | 50.563 | 22.605 | 1.00 | 21.85 | 7 | 353 | O   | MET A  | 45 | 43.011 | 59.512 | 19.985 | 1.00 | 12.88 | 8  |
| 312 | N   | SER A | 41 | 50.307 | 56.831 | 21.475 | 1.00 | 16.33 | 7 | 354 | CB  | MET A  | 45 | 45.028 | 59.874 | 17.442 | 1.00 | 13.26 | 6  |
| 313 | CA  | SER A | 41 | 51.307 | 57.853 | 21.746 | 1.00 | 17.21 | 6 | 355 | CG  | AMET A | 45 | 46.067 | 60.710 | 16.692 | 0.50 | 14.78 | 6  |
| 314 | C   | SER A | 41 | 50.929 | 59.210 | 21.203 | 1.00 | 16.87 | 6 | 356 | SD  | AMET A | 45 | 45.379 | 61.237 | 15.135 | 0.50 | 13.95 | 16 |
| 315 | O   | SER A | 41 | 51.606 | 60.250 | 21.492 | 1.00 | 16.04 | 8 | 357 | CE  | AMET A | 45 | 45.728 | 60.040 | 13.903 | 0.50 | 12.41 | 6  |
| 316 | CB  | SER A | 41 | 52.714 | 57.429 | 21.198 | 1.00 | 17.96 | 6 | 358 | CG  | BMET A | 45 | 45.776 | 60.960 | 16.619 | 0.50 | 11.59 | 6  |
| 317 | OG  | SER A | 41 | 52.625 | 57.387 | 19.782 | 1.00 | 20.42 | 8 | 359 | CA  | TYR A  | 46 | 46.918 | 60.290 | 15.431 | 0.50 | 16.20 | 16 |
| 318 | N   | LYS A | 42 | 49.895 | 59.315 | 20.388 | 1.00 | 13.73 | 7 | 360 | C   | TYR A  | 46 | 45.864 | 59.453 | 14.271 | 0.50 | 18.11 | 6  |
| 319 | CA  | LYS A | 42 | 49.446 | 60.589 | 19.836 | 1.00 | 12.77 | 6 | 361 | O   | TYR A  | 46 | 42.122 | 58.961 | 17.976 | 1.00 | 10.91 | 7  |
| 320 | C   | LYS A | 42 | 48.152 | 60.921 | 20.603 | 1.00 | 13.20 | 6 | 362 | CB  | TYR A  | 46 | 41.356 | 57.880 | 18.584 | 1.00 | 13.29 | 6  |
| 321 | O   | LYS A | 42 | 47.111 | 60.351 | 20.317 | 1.00 | 12.98 | 8 | 363 | C   | TYR A  | 46 | 42.263 | 56.691 | 18.938 | 1.00 | 13.10 | 6  |
| 322 | CB  | LYS A | 42 | 49.193 | 60.477 | 18.321 | 1.00 | 14.60 | 6 | 364 | O   | TYR A  | 46 | 43.076 | 56.318 | 18.094 | 1.00 | 12.46 | 8  |
| 323 | CG  | LYS A | 42 | 50.523 | 60.079 | 17.606 | 1.00 | 19.41 | 6 | 365 | CB  | TYR A  | 46 | 40.258 | 57.364 | 17.660 | 1.00 | 12.44 | 6  |
| 324 | CD  | LYS A | 42 | 50.228 | 60.163 | 16.078 | 1.00 | 25.03 | 6 | 366 | CG  | TYR A  | 46 | 39.031 | 58.210 | 17.416 | 1.00 | 13.02 | 6  |
| 325 | CE  | LYS A | 42 | 51.611 | 60.340 | 15.395 | 1.00 | 34.65 | 6 | 367 | CD1 | TYR A  | 46 | 39.075 | 59.210 | 16.436 | 1.00 | 11.30 | 6  |
| 326 | NZ  | LYS A | 42 | 52.071 | 58.949 | 15.130 | 1.00 | 41.02 | 7 | 368 | CD2 | TYR A  | 46 | 37.846 | 57.978 | 18.105 | 1.00 | 12.45 | 6  |
| 327 | N   | TRP A | 43 | 48.256 | 61.858 | 21.565 | 1.00 | 11.08 | 7 | 369 | CE1 | TYR A  | 46 | 37.940 | 59.997 | 16.146 | 1.00 | 12.75 | 6  |
| 328 | CA  | TRP A | 43 | 47.235 | 61.925 | 22.643 | 1.00 | 13.35 | 6 | 370 | CE2 | TYR A  | 46 | 36.683 | 58.746 | 17.838 | 1.00 | 9.77  | 6  |
| 329 | C   | TRP A | 43 | 45.915 | 62.494 | 22.162 | 1.00 | 11.08 | 6 | 371 | CZ  | TYR A  | 46 | 36.789 | 59.707 | 16.881 | 1.00 | 10.60 | 6  |
| 330 | O   | TRP A | 43 | 45.002 | 62.429 | 22.997 | 1.00 | 13.47 | 8 | 372 | OH  | TYR A  | 46 | 35.703 | 60.490 | 16.547 | 1.00 | 11.65 | 8  |
| 331 | CB  | TRP A | 43 | 47.831 | 62.848 | 23.743 | 1.00 | 14.15 | 6 | 373 | N   | TRP A  | 47 | 42.097 | 56.222 | 20.188 | 1.00 | 9.67  | 7  |
| 332 | CG  | TRP A | 43 | 48.739 | 61.957 | 24.592 | 1.00 | 12.91 | 6 | 374 | CA  | TRP A  | 47 | 42.866 | 55.089 | 20.664 | 1.00 | 11.50 | 6  |
| 333 | CD1 | TRP A | 43 | 50.014 | 61.590 | 24.338 | 1.00 | 14.88 | 6 | 375 | C   | TRP A  | 47 | 42.065 | 53.770 | 20.579 | 1.00 | 12.29 | 6  |
| 334 | CD2 | TRP A | 43 | 48.362 | 61.357 | 25.845 | 1.00 | 12.18 | 6 | 376 | O   | TRP A  | 47 | 42.633 | 52.676 | 20.711 | 1.00 | 12.20 | 8  |
| 335 | NE1 | TRP A | 43 | 50.507 | 60.770 | 25.364 | 1.00 | 16.61 | 7 | 377 | CB  | TRP A  | 47 | 43.430 | 55.285 | 22.077 | 1.00 | 12.80 | 6  |
| 336 | CE2 | TRP A | 43 | 49.467 | 60.633 | 26.297 | 1.00 | 17.08 | 6 | 378 | CG  | TRP A  | 47 | 44.548 | 56.316 | 22.086 | 1.00 | 10.46 | 6  |
| 337 | CE3 | TRP A | 43 | 47.186 | 61.367 | 26.617 | 1.00 | 13.97 | 6 | 379 | CD1 | TRP A  | 47 | 45.068 | 57.007 | 21.037 | 1.00 | 11.88 | 6  |
| 338 | CZ2 | TRP A | 43 | 49.497 | 59.891 | 27.501 | 1.00 | 19.44 | 6 | 380 | CD2 | TRP A  | 47 | 45.300 | 56.687 | 23.218 | 1.00 | 10.01 | 6  |
| 339 | CZ3 | TRP A | 43 | 47.223 | 60.644 | 27.814 | 1.00 | 14.34 | 6 | 381 | NE1 | TRP A  | 47 | 46.060 | 57.853 | 21.485 | 1.00 | 11.36 | 7  |
| 340 | CH2 | TRP A | 43 | 48.333 | 59.925 | 28.265 | 1.00 | 15.92 | 6 | 382 | CE2 | TRP A  | 47 | 46.219 | 57.700 | 22.820 | 1.00 | 12.07 | 6  |
| 341 | N   | LYS A | 44 | 45.846 | 63.088 | 20.972 | 1.00 | 11.78 | 7 | 383 | CE3 | TRP A  | 47 | 45.198 | 56.392 | 24.603 | 1.00 | 12.09 | 6  |
| 342 | CA  | LYS A | 44 | 44.532 | 63.606 | 20.529 | 1.00 | 10.59 | 6 | 384 | CZ2 | TRP A  | 47 | 47.103 | 58.301 | 23.715 | 1.00 | 13.05 | 6  |
| 343 | C   | LYS A | 44 | 43.959 | 62.797 | 19.362 | 1.00 | 11.15 | 6 | 385 | CH2 | TRP A  | 47 | 46.072 | 56.974 | 25.484 | 1.00 | 15.07 | 6  |
| 344 | O   | LYS A | 44 | 43.021 | 63.227 | 18.707 | 1.00 | 11.48 | 8 | 386 | N   | GLY A  | 48 | 47.002 | 57.939 | 25.033 | 1.00 | 16.33 | 6  |
| 345 | CB  | LYS A | 44 | 44.647 | 65.112 | 20.097 | 1.00 | 11.58 | 6 | 387 | CA  | GLY A  | 48 | 40.752 | 53.875 | 20.442 | 1.00 | 10.96 | 7  |
| 346 | CG  | LYS A | 44 | 45.053 | 65.911 | 21.382 | 1.00 | 11.48 | 6 | 388 | C   | GLY A  | 48 | 39.995 | 52.631 | 20.097 | 1.00 | 11.53 | 6  |
| 347 | CD  | LYS A | 44 | 44.928 | 67.435 | 21.011 | 1.00 | 12.19 | 6 | 389 |     |        |    | 38.960 | 52.197 | 21.106 | 1.00 | 11.03 | 6  |

|     |     |       |    |        |        |        |      |       |   |     |     |       |    |        |        |        |      |       |   |
|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| 387 | O   | GLY A | 48 | 38.208 | 51.215 | 20.845 | 1.00 | 12.01 | 8 | 429 | CA  | ARG A | 55 | 29.382 | 46.875 | 28.101 | 1.00 | 13.29 | 6 |
| 388 | N   | GLY A | 49 | 38.834 | 52.862 | 22.221 | 1.00 | 12.42 | 7 | 430 | C   | ARG A | 55 | 30.112 | 45.671 | 28.652 | 1.00 | 12.91 | 6 |
| 389 | CA  | GLY A | 49 | 37.789 | 52.443 | 23.230 | 1.00 | 12.08 | 6 | 431 | O   | ARG A | 55 | 29.684 | 44.943 | 29.596 | 1.00 | 13.96 | 8 |
| 390 | C   | GLY A | 49 | 36.451 | 52.679 | 22.614 | 1.00 | 9.81  | 6 | 432 | CB  | ARG A | 55 | 28.627 | 46.458 | 26.819 | 1.00 | 13.43 | 6 |
| 391 | O   | GLY A | 49 | 36.173 | 53.629 | 21.880 | 1.00 | 10.92 | 8 | 433 | CG  | ARG A | 55 | 27.364 | 45.611 | 27.165 | 1.00 | 13.64 | 6 |
| 392 | N   | ASP A | 50 | 35.433 | 51.851 | 23.065 | 1.00 | 10.42 | 7 | 434 | CD  | ARG A | 55 | 26.723 | 44.974 | 25.877 | 1.00 | 13.15 | 6 |
| 393 | CA  | ASP A | 50 | 34.135 | 51.985 | 22.429 | 1.00 | 11.91 | 6 | 435 | NE  | ARG A | 55 | 27.745 | 44.040 | 25.358 | 1.00 | 13.30 | 7 |
| 394 | C   | ASP A | 50 | 32.977 | 51.516 | 23.344 | 1.00 | 11.85 | 6 | 436 | CZ  | ARG A | 55 | 28.117 | 42.905 | 25.921 | 1.00 | 14.35 | 6 |
| 395 | O   | ASP A | 50 | 33.188 | 51.228 | 24.489 | 1.00 | 12.76 | 8 | 437 | NH1 | ARG A | 55 | 27.475 | 42.404 | 27.011 | 1.00 | 15.82 | 7 |
| 396 | CB  | ASP A | 50 | 34.148 | 51.188 | 21.094 | 1.00 | 10.66 | 6 | 438 | NH2 | ARG A | 55 | 29.125 | 42.171 | 25.446 | 1.00 | 17.12 | 7 |
| 397 | CG  | ASP A | 50 | 34.693 | 49.790 | 21.327 | 1.00 | 14.50 | 6 | 439 | N   | GLN A | 56 | 31.265 | 45.354 | 28.031 | 1.00 | 11.75 | 7 |
| 398 | OD1 | ASP A | 50 | 34.446 | 49.184 | 22.384 | 1.00 | 11.19 | 8 | 440 | CA  | GLN A | 56 | 32.050 | 44.171 | 28.503 | 1.00 | 12.69 | 6 |
| 399 | OD2 | ASP A | 50 | 35.425 | 49.205 | 20.532 | 1.00 | 11.87 | 8 | 441 | C   | GLN A | 56 | 32.530 | 44.339 | 29.945 | 1.00 | 14.76 | 6 |
| 400 | N   | LEU A | 51 | 31.762 | 51.615 | 22.778 | 1.00 | 11.80 | 7 | 442 | O   | GLN A | 56 | 32.895 | 43.338 | 30.611 | 1.00 | 15.16 | 8 |
| 401 | CA  | LEU A | 51 | 30.580 | 51.320 | 23.617 | 1.00 | 11.32 | 6 | 443 | CB  | GLN A | 56 | 33.249 | 43.948 | 27.536 | 1.00 | 12.12 | 6 |
| 402 | C   | LEU A | 51 | 30.568 | 49.843 | 23.973 | 1.00 | 13.43 | 6 | 444 | CG  | GLN A | 56 | 32.718 | 43.310 | 26.223 | 1.00 | 12.45 | 6 |
| 403 | O   | LEU A | 51 | 30.145 | 49.499 | 25.090 | 1.00 | 11.80 | 8 | 445 | CD  | GLN A | 56 | 33.748 | 43.189 | 25.110 | 1.00 | 18.74 | 6 |
| 404 | CB  | LEU A | 51 | 29.272 | 51.662 | 22.869 | 1.00 | 12.03 | 6 | 446 | OE1 | GLN A | 56 | 33.441 | 43.161 | 23.879 | 1.00 | 21.22 | 8 |
| 405 | CG  | LEU A | 51 | 29.178 | 53.205 | 22.638 | 1.00 | 11.71 | 6 | 447 | NE2 | GLN A | 56 | 34.957 | 43.066 | 25.540 | 1.00 | 13.29 | 7 |
| 406 | CD1 | LEU A | 51 | 28.036 | 53.389 | 21.666 | 1.00 | 13.88 | 6 | 448 | N   | LYS A | 57 | 32.816 | 45.574 | 30.355 | 1.00 | 13.93 | 7 |
| 407 | CD2 | LEU A | 51 | 28.915 | 53.930 | 23.954 | 1.00 | 15.76 | 6 | 449 | CA  | LYS A | 57 | 33.243 | 45.881 | 31.703 | 1.00 | 11.77 | 6 |
| 408 | N   | GLU A | 52 | 30.942 | 48.987 | 23.037 | 1.00 | 12.67 | 7 | 450 | C   | LYS A | 57 | 32.146 | 46.200 | 32.702 | 1.00 | 13.05 | 6 |
| 409 | CA  | GLU A | 52 | 30.995 | 47.541 | 23.443 | 1.00 | 12.25 | 6 | 451 | O   | LYS A | 57 | 32.397 | 46.651 | 33.834 | 1.00 | 12.11 | 8 |
| 410 | C   | GLU A | 52 | 32.024 | 47.239 | 24.516 | 1.00 | 12.73 | 6 | 452 | CB  | LYS A | 57 | 34.240 | 47.112 | 31.625 | 1.00 | 12.27 | 6 |
| 411 | O   | GLU A | 52 | 31.816 | 46.375 | 25.382 | 1.00 | 13.32 | 8 | 453 | CG  | LYS A | 57 | 35.508 | 46.752 | 30.818 | 1.00 | 13.15 | 6 |
| 412 | CB  | GLU A | 52 | 31.182 | 46.786 | 22.122 | 1.00 | 16.82 | 6 | 454 | CD  | LYS A | 57 | 36.167 | 45.442 | 31.318 | 1.00 | 13.38 | 6 |
| 413 | CG  | GLU A | 52 | 31.390 | 45.298 | 22.295 | 1.00 | 22.57 | 6 | 455 | CE  | LYS A | 57 | 37.577 | 45.277 | 30.729 | 1.00 | 16.88 | 6 |
| 414 | CD  | GLU A | 52 | 30.227 | 44.545 | 22.992 | 1.00 | 12.69 | 6 | 456 | NZ  | LYS A | 57 | 38.170 | 43.960 | 31.261 | 1.00 | 17.21 | 7 |
| 415 | OE1 | GLU A | 52 | 29.097 | 45.029 | 23.005 | 1.00 | 17.98 | 8 | 457 | N   | LEU A | 58 | 30.883 | 45.891 | 32.388 | 1.00 | 12.90 | 7 |
| 416 | OE2 | GLU A | 52 | 30.680 | 43.475 | 23.419 | 1.00 | 16.49 | 8 | 458 | CA  | LEU A | 58 | 29.789 | 46.048 | 33.338 | 1.00 | 14.31 | 6 |
| 417 | N   | GLY A | 53 | 33.114 | 48.012 | 24.628 | 1.00 | 12.03 | 7 | 459 | C   | LEU A | 58 | 29.981 | 45.299 | 34.668 | 1.00 | 12.68 | 6 |
| 418 | CA  | GLY A | 53 | 34.108 | 47.857 | 25.680 | 1.00 | 13.18 | 6 | 460 | O   | LEU A | 58 | 29.737 | 45.865 | 35.732 | 1.00 | 13.94 | 8 |
| 419 | C   | GLY A | 53 | 33.471 | 48.292 | 27.005 | 1.00 | 12.67 | 6 | 461 | CB  | LEU A | 58 | 28.407 | 45.779 | 32.723 | 1.00 | 12.52 | 6 |
| 420 | O   | GLY A | 53 | 33.737 | 47.586 | 28.000 | 1.00 | 11.91 | 8 | 462 | CG  | LEU A | 58 | 27.963 | 46.878 | 31.718 | 1.00 | 12.14 | 6 |
| 421 | N   | VAL A | 54 | 32.653 | 49.355 | 27.005 | 1.00 | 11.80 | 7 | 463 | CD1 | LEU A | 58 | 26.709 | 46.366 | 30.943 | 1.00 | 14.87 | 6 |
| 422 | CA  | VAL A | 54 | 31.996 | 49.680 | 28.280 | 1.00 | 10.05 | 6 | 464 | CD2 | LEU A | 58 | 27.586 | 48.136 | 32.488 | 1.00 | 15.84 | 6 |
| 423 | C   | VAL A | 54 | 31.078 | 48.502 | 28.715 | 1.00 | 12.37 | 6 | 465 | N   | PRO A | 59 | 30.555 | 44.107 | 34.670 | 1.00 | 13.13 | 7 |
| 424 | O   | VAL A | 54 | 31.055 | 48.111 | 29.879 | 1.00 | 12.15 | 8 | 466 | CA  | PRO A | 59 | 30.776 | 43.396 | 35.937 | 1.00 | 14.64 | 6 |
| 425 | CB  | VAL A | 54 | 31.154 | 50.947 | 28.220 | 1.00 | 11.03 | 6 | 467 | C   | PRO A | 59 | 31.759 | 44.139 | 36.827 | 1.00 | 14.63 | 6 |
| 426 | CG1 | VAL A | 54 | 30.449 | 51.255 | 29.552 | 1.00 | 13.86 | 6 | 468 | O   | PRO A | 59 | 31.532 | 44.250 | 38.038 | 1.00 | 15.79 | 8 |
| 427 | CG2 | VAL A | 54 | 32.100 | 52.143 | 27.853 | 1.00 | 11.86 | 6 | 469 | CB  | PRO A | 59 | 31.436 | 42.034 | 35.525 | 1.00 | 15.40 | 6 |
| 428 | N   | ARG A | 55 | 30.387 | 47.952 | 27.708 | 1.00 | 9.95  | 7 | 470 | CG  | PRO A | 59 | 30.719 | 41.845 | 34.161 | 1.00 | 16.79 | 6 |



|     |     |     |   |    |        |        |        |      |       |   |     |     |     |   |    |        |        |        |      |       |   |
|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 550 | CD1 | ILE | A | 69 | 27.937 | 52.008 | 32.775 | 1.00 | 13.93 | 6 | 592 | CG2 | VAL | A | 74 | 25.882 | 58.894 | 22.161 | 1.00 | 10.26 | 6 |
| 551 | N   | TRP | A | 70 | 28.196 | 57.872 | 33.425 | 1.00 | 9.74  | 7 | 593 | N   | LEU | A | 75 | 27.708 | 60.912 | 19.980 | 1.00 | 10.62 | 7 |
| 552 | CA  | TRP | A | 70 | 28.095 | 59.093 | 32.600 | 1.00 | 10.34 | 6 | 594 | CA  | LEU | A | 75 | 27.182 | 61.136 | 18.619 | 1.00 | 10.48 | 6 |
| 553 | C   | TRP | A | 70 | 28.991 | 58.790 | 31.403 | 1.00 | 11.63 | 6 | 595 | C   | LEU | A | 75 | 28.305 | 61.464 | 17.620 | 1.00 | 12.02 | 6 |
| 554 | O   | TRP | A | 70 | 30.214 | 58.751 | 31.558 | 1.00 | 11.51 | 8 | 596 | O   | LEU | A | 75 | 29.436 | 61.678 | 18.016 | 1.00 | 11.28 | 8 |
| 555 | CB  | TRP | A | 70 | 28.494 | 60.327 | 33.441 | 1.00 | 9.83  | 6 | 597 | CB  | LEU | A | 75 | 26.111 | 62.279 | 18.660 | 1.00 | 10.81 | 6 |
| 556 | CG  | TRP | A | 70 | 28.954 | 61.558 | 32.738 | 1.00 | 8.81  | 6 | 598 | CG  | LEU | A | 75 | 24.952 | 61.966 | 19.634 | 1.00 | 11.49 | 6 |
| 557 | CD1 | TRP | A | 70 | 29.050 | 61.770 | 31.360 | 1.00 | 13.03 | 6 | 599 | CD1 | LEU | A | 75 | 24.074 | 63.178 | 19.911 | 1.00 | 11.47 | 6 |
| 558 | CD2 | TRP | A | 70 | 29.591 | 62.698 | 33.356 | 1.00 | 10.57 | 6 | 600 | CD2 | LEU | A | 75 | 24.074 | 60.864 | 18.960 | 1.00 | 11.05 | 6 |
| 559 | NE1 | TRP | A | 70 | 29.645 | 63.016 | 31.118 | 1.00 | 12.41 | 7 | 601 | N   | ASP | A | 76 | 27.958 | 61.296 | 16.347 | 1.00 | 10.11 | 7 |
| 560 | CE2 | TRP | A | 70 | 30.017 | 63.558 | 32.338 | 1.00 | 10.48 | 6 | 602 | CA  | ASP | A | 76 | 29.020 | 61.292 | 15.299 | 1.00 | 9.23  | 6 |
| 561 | CE3 | TRP | A | 70 | 29.830 | 63.007 | 34.699 | 1.00 | 12.18 | 6 | 603 | C   | ASP | A | 76 | 29.821 | 62.605 | 15.351 | 1.00 | 9.60  | 6 |
| 562 | CZ2 | TRP | A | 70 | 30.721 | 64.729 | 32.587 | 1.00 | 9.61  | 6 | 604 | O   | ASP | A | 76 | 29.263 | 63.683 | 15.155 | 1.00 | 11.11 | 8 |
| 563 | CZ3 | TRP | A | 70 | 30.426 | 64.234 | 34.950 | 1.00 | 11.62 | 6 | 605 | CB  | ASP | A | 76 | 28.264 | 61.153 | 13.979 | 1.00 | 9.89  | 6 |
| 564 | CH2 | TRP | A | 70 | 30.896 | 65.061 | 33.914 | 1.00 | 13.98 | 6 | 606 | CG  | ASP | A | 76 | 29.177 | 61.079 | 12.745 | 1.00 | 12.56 | 6 |
| 565 | N   | LEU | A | 71 | 28.373 | 58.542 | 30.225 | 1.00 | 10.83 | 7 | 607 | OD1 | ASP | A | 76 | 30.380 | 60.856 | 12.895 | 1.00 | 12.97 | 8 |
| 566 | CA  | LEU | A | 71 | 29.219 | 58.311 | 29.023 | 1.00 | 11.92 | 6 | 608 | OD2 | ASP | A | 76 | 28.617 | 61.239 | 11.641 | 1.00 | 11.97 | 8 |
| 567 | C   | LEU | A | 71 | 29.585 | 59.691 | 28.439 | 1.00 | 10.49 | 6 | 609 | N   | ASN | A | 77 | 31.131 | 62.435 | 15.524 | 1.00 | 9.80  | 7 |
| 568 | O   | LEU | A | 71 | 28.669 | 60.552 | 28.276 | 1.00 | 10.64 | 8 | 610 | CA  | ASN | A | 77 | 32.043 | 63.570 | 15.534 | 1.00 | 9.86  | 6 |
| 569 | CB  | LEU | A | 71 | 28.342 | 57.617 | 27.923 | 1.00 | 11.13 | 6 | 611 | C   | ASN | A | 77 | 32.766 | 63.691 | 14.180 | 1.00 | 10.69 | 6 |
| 570 | CG  | LEU | A | 71 | 27.991 | 56.159 | 28.240 | 1.00 | 11.31 | 6 | 612 | O   | ASN | A | 77 | 32.797 | 62.759 | 13.385 | 1.00 | 10.51 | 8 |
| 571 | CD1 | LEU | A | 71 | 27.073 | 55.665 | 27.096 | 1.00 | 10.98 | 6 | 613 | CB  | ASN | A | 77 | 33.117 | 63.370 | 16.619 | 1.00 | 10.13 | 6 |
| 572 | CD2 | LEU | A | 71 | 29.253 | 55.314 | 28.322 | 1.00 | 11.96 | 6 | 614 | CG  | ASN | A | 77 | 32.685 | 63.988 | 17.945 | 1.00 | 13.40 | 6 |
| 573 | N   | SER | A | 72 | 30.870 | 59.865 | 28.066 | 1.00 | 10.17 | 7 | 615 | OD1 | ASN | A | 77 | 33.515 | 64.636 | 18.600 | 1.00 | 10.92 | 8 |
| 574 | CA  | SER | A | 72 | 31.250 | 60.995 | 27.218 | 1.00 | 9.81  | 6 | 616 | ND2 | ASN | A | 77 | 31.412 | 63.908 | 18.341 | 1.00 | 11.73 | 7 |
| 575 | C   | SER | A | 72 | 30.455 | 60.988 | 25.920 | 1.00 | 11.22 | 6 | 617 | N   | LEU | A | 78 | 33.296 | 64.886 | 13.967 | 1.00 | 10.62 | 7 |
| 576 | O   | SER | A | 72 | 29.733 | 60.011 | 25.572 | 1.00 | 10.33 | 8 | 618 | CA  | LEU | A | 78 | 34.240 | 65.195 | 12.866 | 1.00 | 11.24 | 6 |
| 577 | CB  | SER | A | 72 | 32.773 | 60.898 | 26.944 | 1.00 | 10.62 | 6 | 619 | C   | LEU | A | 78 | 34.929 | 63.977 | 12.309 | 1.00 | 8.87  | 6 |
| 578 | OG  | SER | A | 72 | 33.092 | 59.694 | 26.237 | 1.00 | 11.62 | 8 | 620 | O   | LEU | A | 78 | 35.632 | 63.257 | 13.026 | 1.00 | 12.04 | 8 |
| 579 | N   | PRO | A | 73 | 30.447 | 62.034 | 25.128 | 1.00 | 11.10 | 7 | 621 | CB  | LEU | A | 78 | 35.257 | 66.197 | 13.506 | 1.00 | 9.81  | 6 |
| 580 | CA  | PRO | A | 73 | 29.427 | 62.188 | 24.048 | 1.00 | 11.86 | 6 | 622 | CG  | LEU | A | 78 | 36.289 | 66.679 | 12.399 | 1.00 | 9.30  | 6 |
| 581 | C   | PRO | A | 73 | 29.521 | 61.057 | 23.042 | 1.00 | 13.54 | 6 | 623 | CD1 | LEU | A | 78 | 35.622 | 67.597 | 11.418 | 1.00 | 11.34 | 6 |
| 582 | O   | PRO | A | 73 | 30.653 | 60.649 | 22.674 | 1.00 | 11.75 | 8 | 624 | CD2 | LEU | A | 78 | 37.382 | 67.439 | 13.176 | 1.00 | 13.04 | 6 |
| 583 | CB  | PRO | A | 73 | 29.672 | 63.563 | 23.414 | 1.00 | 10.32 | 6 | 625 | N   | ASP | A | 79 | 34.801 | 63.867 | 10.945 | 1.00 | 11.36 | 7 |
| 584 | CG  | PRO | A | 73 | 30.360 | 64.313 | 24.557 | 1.00 | 10.23 | 6 | 626 | CA  | ASP | A | 79 | 35.393 | 62.670 | 10.348 | 1.00 | 9.32  | 6 |
| 585 | CD  | PRO | A | 73 | 31.228 | 63.286 | 25.358 | 1.00 | 11.09 | 6 | 627 | C   | ASP | A | 79 | 36.754 | 62.947 | 9.688  | 1.00 | 12.70 | 6 |
| 586 | N   | VAL | A | 74 | 28.345 | 60.538 | 22.623 | 1.00 | 11.02 | 7 | 628 | O   | ASP | A | 79 | 37.275 | 62.042 | 9.026  | 1.00 | 14.30 | 8 |
| 587 | CA  | VAL | A | 74 | 28.351 | 59.338 | 21.794 | 1.00 | 9.14  | 6 | 629 | CB  | ASP | A | 79 | 34.468 | 62.189 | 9.168  | 1.00 | 14.19 | 6 |
| 588 | C   | VAL | A | 74 | 27.998 | 59.628 | 20.344 | 1.00 | 9.79  | 6 | 630 | CG  | ASP | A | 79 | 33.217 | 61.518 | 9.658  | 1.00 | 15.14 | 6 |
| 589 | O   | VAL | A | 74 | 28.041 | 58.700 | 19.549 | 1.00 | 10.96 | 8 | 631 | OD1 | ASP | A | 79 | 33.208 | 61.150 | 10.841 | 1.00 | 12.50 | 8 |
| 590 | CB  | VAL | A | 74 | 27.260 | 58.313 | 22.311 | 1.00 | 9.29  | 6 | 632 | OD2 | ASP | A | 79 | 32.239 | 61.307 | 8.931  | 1.00 | 12.26 | 8 |
| 591 | CG1 | VAL | A | 74 | 27.541 | 57.935 | 23.780 | 1.00 | 11.66 | 6 | 633 | N   | THR | A | 80 | 37.307 | 64.115 | 9.950  | 1.00 | 12.57 | 7 |







|     |     |           |        |        |        |      |       |   |     |     |           |        |        |        |      |       |   |
|-----|-----|-----------|--------|--------|--------|------|-------|---|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 802 | CB  | ILE A 100 | 26.080 | 55.834 | 17.385 | 1.00 | 11.20 | 6 | 844 | CZ  | PHE A 104 | 34.365 | 58.005 | 21.053 | 1.00 | 13.46 | 6 |
| 803 | CG1 | ILE A 100 | 24.767 | 55.651 | 18.197 | 1.00 | 13.05 | 6 | 845 | N   | GLY A 105 | 30.491 | 52.584 | 17.759 | 1.00 | 14.42 | 7 |
| 804 | CG2 | ILE A 100 | 27.229 | 55.284 | 18.240 | 1.00 | 10.14 | 6 | 846 | CA  | GLY A 105 | 29.462 | 51.533 | 17.546 | 1.00 | 16.52 | 6 |
| 805 | CD1 | ILE A 100 | 24.692 | 56.541 | 19.489 | 1.00 | 13.82 | 6 | 847 | C   | GLY A 105 | 28.362 | 52.143 | 16.670 | 1.00 | 17.63 | 6 |
| 806 | N   | GLU A 101 | 28.607 | 57.861 | 16.898 | 1.00 | 11.66 | 7 | 848 | O   | GLY A 105 | 28.624 | 53.104 | 15.927 | 1.00 | 14.43 | 8 |
| 807 | CA  | GLU A 101 | 29.968 | 57.886 | 16.322 | 1.00 | 11.19 | 6 | 849 | N   | ASN A 106 | 27.169 | 51.558 | 16.664 | 1.00 | 14.15 | 7 |
| 808 | C   | GLU A 101 | 30.443 | 56.478 | 15.956 | 1.00 | 11.88 | 6 | 850 | CA  | ASN A 106 | 26.017 | 52.150 | 15.960 | 1.00 | 11.27 | 6 |
| 809 | O   | GLU A 101 | 30.430 | 55.545 | 16.758 | 1.00 | 12.38 | 8 | 851 | C   | ASN A 106 | 24.864 | 52.149 | 16.958 | 1.00 | 13.27 | 6 |
| 810 | CB  | GLU A 101 | 30.918 | 58.478 | 17.400 | 1.00 | 11.53 | 6 | 852 | O   | ASN A 106 | 25.081 | 51.890 | 18.174 | 1.00 | 13.00 | 8 |
| 811 | CG  | GLU A 101 | 32.427 | 58.256 | 17.126 | 1.00 | 10.12 | 6 | 853 | CB  | ASN A 106 | 25.756 | 51.332 | 14.677 | 1.00 | 13.55 | 6 |
| 812 | CD  | GLU A 101 | 32.796 | 58.791 | 15.715 | 1.00 | 10.82 | 6 | 854 | CG  | ASN A 106 | 25.465 | 49.876 | 14.958 | 1.00 | 18.28 | 6 |
| 813 | OE1 | GLU A 101 | 32.328 | 59.903 | 15.389 | 1.00 | 11.74 | 8 | 855 | OD1 | ASN A 106 | 25.093 | 49.459 | 16.033 | 1.00 | 17.05 | 8 |
| 814 | OE2 | GLU A 101 | 33.577 | 58.059 | 15.099 | 1.00 | 12.29 | 8 | 856 | ND2 | ASN A 106 | 25.576 | 49.021 | 13.910 | 1.00 | 22.96 | 7 |
| 815 | N   | GLU A 102 | 30.874 | 56.411 | 14.662 | 1.00 | 12.51 | 7 | 857 | N   | TRP A 107 | 23.668 | 52.508 | 16.525 | 1.00 | 12.62 | 7 |
| 816 | CA  | GLU A 102 | 31.192 | 55.081 | 14.116 | 1.00 | 11.29 | 6 | 858 | CA  | TRP A 107 | 22.554 | 52.559 | 17.465 | 1.00 | 13.67 | 6 |
| 817 | C   | GLU A 102 | 32.387 | 54.443 | 14.766 | 1.00 | 12.50 | 6 | 859 | C   | TRP A 107 | 22.296 | 51.203 | 18.121 | 1.00 | 14.10 | 6 |
| 818 | O   | GLU A 102 | 32.460 | 53.176 | 14.813 | 1.00 | 11.57 | 8 | 860 | O   | TRP A 107 | 21.827 | 51.121 | 19.274 | 1.00 | 14.66 | 8 |
| 819 | CB  | GLU A 102 | 31.402 | 55.182 | 12.553 | 1.00 | 11.80 | 6 | 861 | CB  | TRP A 107 | 21.268 | 53.087 | 16.802 | 1.00 | 14.53 | 6 |
| 820 | CG  | GLU A 102 | 32.656 | 55.982 | 12.107 | 1.00 | 12.52 | 6 | 862 | CB  | TRP A 107 | 21.256 | 54.576 | 16.836 | 1.00 | 16.29 | 6 |
| 821 | CD  | GLU A 102 | 32.465 | 57.475 | 12.181 | 1.00 | 12.69 | 6 | 863 | CD1 | TRP A 107 | 21.351 | 55.357 | 15.696 | 1.00 | 17.56 | 6 |
| 822 | OE1 | GLU A 102 | 31.368 | 58.018 | 12.431 | 1.00 | 14.09 | 8 | 864 | CD2 | TRP A 107 | 21.131 | 55.454 | 17.949 | 1.00 | 15.71 | 6 |
| 823 | OE2 | GLU A 102 | 33.493 | 58.174 | 11.930 | 1.00 | 15.94 | 8 | 865 | NE1 | TRP A 107 | 21.279 | 56.677 | 16.088 | 1.00 | 16.73 | 7 |
| 824 | N   | HIS A 103 | 33.391 | 55.145 | 15.324 | 1.00 | 9.73  | 7 | 866 | CE2 | TRP A 107 | 21.186 | 56.759 | 17.451 | 1.00 | 14.24 | 6 |
| 825 | CA  | HIS A 103 | 34.429 | 54.494 | 16.120 | 1.00 | 9.99  | 6 | 867 | CE3 | TRP A 107 | 20.995 | 55.256 | 19.345 | 1.00 | 13.30 | 6 |
| 826 | C   | HIS A 103 | 33.862 | 53.874 | 17.376 | 1.00 | 11.88 | 6 | 868 | CZ2 | TRP A 107 | 21.082 | 57.915 | 18.240 | 1.00 | 14.74 | 6 |
| 827 | O   | HIS A 103 | 34.531 | 52.943 | 17.864 | 1.00 | 12.86 | 8 | 869 | CZ3 | TRP A 107 | 20.919 | 56.410 | 20.131 | 1.00 | 16.80 | 6 |
| 828 | CB  | HIS A 103 | 35.470 | 55.578 | 16.584 | 1.00 | 12.93 | 6 | 870 | CH2 | TRP A 107 | 20.927 | 57.717 | 19.596 | 1.00 | 13.00 | 6 |
| 829 | CG  | HIS A 103 | 36.364 | 56.049 | 15.481 | 1.00 | 11.28 | 6 | 871 | N   | THR A 108 | 22.439 | 50.097 | 17.351 | 1.00 | 14.29 | 7 |
| 830 | ND1 | HIS A 103 | 36.015 | 57.085 | 14.639 | 1.00 | 12.54 | 7 | 872 | CA  | THR A 108 | 22.316 | 48.792 | 18.020 | 1.00 | 14.34 | 6 |
| 831 | CD2 | HIS A 103 | 37.595 | 55.655 | 15.123 | 1.00 | 14.43 | 6 | 873 | C   | THR A 108 | 23.305 | 48.617 | 19.154 | 1.00 | 16.18 | 6 |
| 832 | CE1 | HIS A 103 | 37.021 | 57.288 | 13.749 | 1.00 | 13.58 | 6 | 874 | O   | THR A 108 | 22.945 | 48.095 | 20.224 | 1.00 | 14.57 | 8 |
| 833 | NE2 | HIS A 103 | 37.965 | 56.434 | 14.054 | 1.00 | 13.95 | 7 | 875 | CB  | THR A 108 | 22.508 | 47.669 | 16.969 | 1.00 | 16.38 | 6 |
| 834 | N   | PHE A 104 | 32.662 | 54.253 | 17.819 | 1.00 | 9.60  | 7 | 876 | OG1 | THR A 108 | 21.473 | 47.841 | 16.005 | 1.00 | 18.39 | 8 |
| 835 | CA  | PHE A 104 | 32.171 | 53.727 | 19.103 | 1.00 | 10.30 | 6 | 877 | CG2 | THR A 108 | 22.386 | 46.276 | 17.600 | 1.00 | 20.41 | 6 |
| 836 | C   | PHE A 104 | 31.116 | 52.625 | 18.924 | 1.00 | 13.76 | 6 | 878 | N   | THR A 109 | 24.581 | 49.043 | 18.959 | 1.00 | 12.36 | 7 |
| 837 | O   | PHE A 104 | 30.969 | 51.851 | 19.894 | 1.00 | 13.23 | 8 | 879 | CA  | THR A 109 | 25.556 | 48.897 | 20.029 | 1.00 | 13.35 | 6 |
| 838 | CB  | PHE A 104 | 31.583 | 54.855 | 19.953 | 1.00 | 10.00 | 6 | 880 | C   | THR A 109 | 25.149 | 49.732 | 21.248 | 1.00 | 12.11 | 6 |
| 839 | CG  | PHE A 104 | 32.587 | 55.933 | 20.330 | 1.00 | 13.59 | 6 | 881 | O   | THR A 109 | 25.318 | 49.282 | 22.382 | 1.00 | 12.78 | 8 |
| 840 | CD1 | PHE A 104 | 33.954 | 55.782 | 20.204 | 1.00 | 11.92 | 6 | 882 | CB  | THR A 109 | 26.960 | 49.404 | 19.545 | 1.00 | 13.85 | 6 |
| 841 | CD2 | PHE A 104 | 32.082 | 57.130 | 20.834 | 1.00 | 13.49 | 6 | 883 | OG1 | THR A 109 | 27.201 | 49.021 | 18.155 | 1.00 | 14.22 | 8 |
| 842 | CE1 | PHE A 104 | 34.854 | 56.802 | 20.561 | 1.00 | 12.32 | 6 | 884 | CG2 | THR A 109 | 28.048 | 48.783 | 20.429 | 1.00 | 15.14 | 6 |
| 843 | CE2 | PHE A 104 | 32.981 | 58.161 | 21.193 | 1.00 | 11.48 | 6 | 885 | N   | PHE A 110 | 24.673 | 50.945 | 20.982 | 1.00 | 12.96 | 7 |

|     |     |           |        |        |        |      |       |   |     |     |           |        |        |        |      |       |   |
|-----|-----|-----------|--------|--------|--------|------|-------|---|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 886 | CA  | PHE A 110 | 24.247 | 51.800 | 22.126 | 1.00 | 12.43 | 6 | 928 | C   | ASN A 115 | 20.678 | 46.553 | 28.961 | 1.00 | 12.99 | 6 |
| 887 | C   | PHE A 110 | 23.058 | 51.137 | 22.830 | 1.00 | 13.48 | 6 | 929 | O   | ASN A 115 | 20.121 | 46.160 | 29.987 | 1.00 | 15.11 | 8 |
| 888 | O   | PHE A 110 | 23.061 | 51.036 | 24.060 | 1.00 | 12.36 | 8 | 930 | CB  | ASN A 115 | 19.372 | 46.637 | 26.820 | 1.00 | 15.99 | 6 |
| 889 | CB  | PHE A 110 | 23.823 | 53.160 | 21.525 | 1.00 | 14.28 | 6 | 931 | CG  | ASN A 115 | 18.200 | 47.261 | 26.118 | 1.00 | 22.41 | 6 |
| 890 | CG  | PHE A 110 | 23.320 | 54.128 | 22.611 | 1.00 | 15.08 | 6 | 932 | OD1 | ASN A 115 | 18.061 | 47.131 | 24.868 | 1.00 | 26.38 | 8 |
| 891 | CD1 | PHE A 110 | 24.190 | 54.941 | 23.252 | 1.00 | 13.29 | 6 | 933 | ND2 | ASN A 115 | 17.304 | 47.937 | 26.823 | 1.00 | 22.30 | 7 |
| 892 | CD2 | PHE A 110 | 21.975 | 54.202 | 22.913 | 1.00 | 14.29 | 6 | 934 | N   | ASP A 116 | 21.940 | 46.229 | 28.669 | 1.00 | 12.94 | 7 |
| 893 | CE1 | PHE A 110 | 23.764 | 55.850 | 24.247 | 1.00 | 13.20 | 6 | 935 | CA  | ASP A 116 | 22.731 | 45.386 | 29.561 | 1.00 | 12.20 | 6 |
| 894 | CE2 | PHE A 110 | 21.487 | 55.055 | 23.876 | 1.00 | 12.89 | 6 | 936 | C   | ASP A 116 | 23.087 | 46.144 | 30.835 | 1.00 | 12.69 | 6 |
| 895 | CZ  | PHE A 110 | 22.377 | 55.898 | 24.558 | 1.00 | 13.20 | 6 | 937 | O   | ASP A 116 | 23.070 | 45.584 | 31.933 | 1.00 | 12.40 | 8 |
| 896 | N   | ASP A 111 | 22.056 | 50.645 | 22.065 | 1.00 | 13.15 | 7 | 938 | CB  | ASP A 116 | 23.989 | 44.814 | 28.887 | 1.00 | 13.19 | 6 |
| 897 | CA  | ASP A 111 | 20.916 | 49.993 | 22.755 | 1.00 | 12.63 | 6 | 939 | CG  | ASP A 116 | 23.648 | 43.698 | 27.896 | 1.00 | 19.33 | 6 |
| 898 | C   | ASP A 111 | 21.337 | 48.770 | 23.517 | 1.00 | 14.08 | 6 | 940 | OD1 | ASP A 116 | 22.461 | 43.487 | 27.582 | 1.00 | 23.80 | 8 |
| 899 | O   | ASP A 111 | 20.917 | 48.606 | 24.698 | 1.00 | 14.41 | 8 | 941 | OD2 | ASP A 116 | 24.583 | 42.967 | 27.460 | 1.00 | 22.90 | 8 |
| 900 | CB  | ASP A 111 | 19.966 | 49.513 | 21.610 | 1.00 | 13.40 | 6 | 942 | N   | ALA A 117 | 23.342 | 47.453 | 30.753 | 1.00 | 12.25 | 7 |
| 901 | CG  | ASP A 111 | 19.224 | 50.603 | 20.937 | 1.00 | 18.96 | 6 | 943 | CA  | ALA A 117 | 23.561 | 48.208 | 32.005 | 1.00 | 12.13 | 6 |
| 902 | OD1 | ASP A 111 | 19.343 | 51.768 | 21.305 | 1.00 | 17.72 | 8 | 944 | C   | ALA A 117 | 22.314 | 48.146 | 32.878 | 1.00 | 10.66 | 6 |
| 903 | OD2 | ASP A 111 | 18.498 | 50.291 | 19.945 | 1.00 | 18.78 | 8 | 945 | O   | ALA A 117 | 22.425 | 47.887 | 34.083 | 1.00 | 12.92 | 8 |
| 904 | N   | THR A 112 | 22.284 | 48.006 | 22.997 | 1.00 | 13.38 | 7 | 946 | CB  | ALA A 117 | 23.877 | 49.692 | 31.625 | 1.00 | 13.05 | 6 |
| 905 | CA  | THR A 112 | 22.756 | 46.828 | 23.771 | 1.00 | 14.87 | 6 | 947 | N   | HIS A 118 | 21.149 | 48.403 | 32.291 | 1.00 | 12.02 | 7 |
| 906 | C   | THR A 112 | 23.450 | 47.184 | 25.017 | 1.00 | 14.48 | 6 | 948 | CA  | HIS A 118 | 19.948 | 48.334 | 33.131 | 1.00 | 10.66 | 6 |
| 907 | O   | THR A 112 | 23.224 | 46.583 | 26.069 | 1.00 | 15.04 | 8 | 949 | C   | HIS A 118 | 19.727 | 46.929 | 33.683 | 1.00 | 12.65 | 6 |
| 908 | CB  | THR A 112 | 23.680 | 45.966 | 22.829 | 1.00 | 15.99 | 6 | 950 | O   | HIS A 118 | 19.267 | 46.870 | 34.838 | 1.00 | 14.87 | 8 |
| 909 | OG1 | THR A 112 | 22.844 | 45.644 | 21.711 | 1.00 | 16.67 | 8 | 951 | CB  | HIS A 118 | 18.714 | 48.622 | 32.200 | 1.00 | 10.79 | 6 |
| 910 | CG2 | THR A 112 | 24.006 | 44.662 | 23.576 | 1.00 | 18.86 | 6 | 952 | CG  | HIS A 118 | 18.691 | 50.088 | 31.789 | 1.00 | 11.37 | 6 |
| 911 | N   | LEU A 113 | 24.321 | 48.221 | 24.968 | 1.00 | 11.85 | 7 | 953 | ND1 | HIS A 118 | 17.881 | 50.557 | 30.773 | 1.00 | 14.86 | 7 |
| 912 | CA  | LEU A 113 | 24.982 | 48.631 | 26.219 | 1.00 | 12.44 | 6 | 954 | CD2 | HIS A 118 | 19.340 | 51.157 | 32.359 | 1.00 | 13.69 | 6 |
| 913 | C   | LEU A 113 | 23.992 | 49.138 | 27.242 | 1.00 | 12.26 | 6 | 955 | CE1 | HIS A 118 | 18.020 | 51.897 | 30.708 | 1.00 | 15.91 | 6 |
| 914 | O   | LEU A 113 | 24.057 | 48.793 | 28.403 | 1.00 | 12.86 | 8 | 956 | NE2 | HIS A 118 | 18.912 | 52.260 | 31.644 | 1.00 | 11.99 | 7 |
| 915 | CB  | LEU A 113 | 25.988 | 49.772 | 25.811 | 1.00 | 10.14 | 6 | 957 | N   | GLN A 119 | 20.028 | 45.871 | 32.935 | 1.00 | 11.93 | 7 |
| 916 | CG  | LEU A 113 | 26.404 | 50.629 | 27.037 | 1.00 | 13.26 | 6 | 958 | CA  | GLN A 119 | 19.843 | 44.545 | 33.592 | 1.00 | 12.22 | 6 |
| 917 | CD1 | LEU A 113 | 27.184 | 49.772 | 28.040 | 1.00 | 13.59 | 6 | 959 | C   | GLN A 119 | 20.770 | 44.412 | 34.781 | 1.00 | 15.02 | 6 |
| 918 | CD2 | LEU A 113 | 27.295 | 51.825 | 26.664 | 1.00 | 12.75 | 6 | 960 | O   | GLN A 119 | 20.519 | 43.615 | 35.694 | 1.00 | 15.33 | 8 |
| 919 | N   | VAL A 114 | 23.020 | 49.971 | 26.823 | 1.00 | 11.82 | 7 | 961 | CB  | GLN A 119 | 20.340 | 43.445 | 32.620 | 1.00 | 16.20 | 6 |
| 920 | CA  | VAL A 114 | 22.073 | 50.545 | 27.762 | 1.00 | 12.84 | 6 | 962 | CG  | GLN A 119 | 19.327 | 43.169 | 31.521 | 1.00 | 17.09 | 6 |
| 921 | C   | VAL A 114 | 21.215 | 49.449 | 28.384 | 1.00 | 13.48 | 6 | 963 | CD  | GLN A 119 | 20.028 | 41.969 | 30.765 | 1.00 | 21.33 | 6 |
| 922 | O   | VAL A 114 | 20.973 | 49.402 | 29.577 | 1.00 | 13.54 | 8 | 964 | OE1 | GLN A 119 | 20.575 | 41.051 | 31.363 | 1.00 | 29.71 | 8 |
| 923 | CB  | VAL A 114 | 21.264 | 51.680 | 27.090 | 1.00 | 13.71 | 6 | 965 | NE2 | GLN A 119 | 19.985 | 42.085 | 29.522 | 1.00 | 20.93 | 7 |
| 924 | CG1 | VAL A 114 | 20.144 | 52.091 | 28.032 | 1.00 | 18.18 | 6 | 966 | N   | ASN A 120 | 21.939 | 45.127 | 34.806 | 1.00 | 15.33 | 7 |
| 925 | CG2 | VAL A 114 | 22.209 | 52.885 | 26.815 | 1.00 | 15.06 | 6 | 967 | CA  | ASN A 120 | 22.853 | 45.072 | 35.932 | 1.00 | 16.39 | 6 |
| 926 | N   | ASN A 115 | 20.760 | 48.534 | 27.512 | 1.00 | 13.50 | 7 | 968 | C   | ASN A 120 | 22.541 | 46.148 | 36.970 | 1.00 | 14.25 | 6 |
| 927 | CA  | ASN A 115 | 19.912 | 47.430 | 28.013 | 1.00 | 11.60 | 6 | 969 | O   | ASN A 120 | 23.358 | 46.337 | 37.876 | 1.00 | 15.65 | 8 |

|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 970  | CB  | ASN A 120 | 24.337 | 45.189 | 35.481 | 1.00 | 12.26 | 6 | 1012 | C   | VAL A 126 | 25.247 | 62.207 | 28.081 | 1.00 | 12.61 | 6 |
| 971  | CG  | ASN A 120 | 24.753 | 43.901 | 34.799 | 1.00 | 20.80 | 6 | 1013 | O   | VAL A 126 | 24.413 | 63.080 | 28.254 | 1.00 | 11.41 | 8 |
| 972  | OD1 | ASN A 120 | 24.778 | 43.805 | 33.576 | 1.00 | 23.34 | 8 | 1014 | CB  | VAL A 126 | 24.039 | 60.356 | 26.823 | 1.00 | 11.44 | 6 |
| 973  | ND2 | ASN A 120 | 25.076 | 42.912 | 35.627 | 1.00 | 18.29 | 7 | 1015 | CG1 | VAL A 126 | 24.892 | 60.704 | 25.575 | 1.00 | 12.92 | 6 |
| 974  | N   | GLY A 121 | 21.398 | 46.801 | 36.951 | 1.00 | 13.35 | 7 | 1016 | CG2 | VAL A 126 | 23.704 | 58.883 | 26.856 | 1.00 | 11.52 | 6 |
| 975  | CA  | GLY A 121 | 20.994 | 47.834 | 37.885 | 1.00 | 16.91 | 6 | 1017 | N   | ASP A 127 | 26.535 | 62.445 | 27.771 | 1.00 | 8.46  | 7 |
| 976  | C   | GLY A 121 | 21.840 | 49.129 | 37.772 | 1.00 | 13.99 | 6 | 1018 | CA  | ASP A 127 | 27.011 | 63.870 | 27.661 | 1.00 | 9.67  | 6 |
| 977  | O   | GLY A 121 | 21.866 | 49.890 | 38.747 | 1.00 | 15.35 | 8 | 1019 | C   | ASP A 127 | 26.509 | 64.374 | 26.283 | 1.00 | 10.71 | 6 |
| 978  | N   | ILE A 122 | 22.262 | 49.397 | 36.527 | 1.00 | 12.67 | 7 | 1020 | O   | ASP A 127 | 26.837 | 63.710 | 25.279 | 1.00 | 11.36 | 8 |
| 979  | CA  | ILE A 122 | 23.128 | 50.569 | 36.322 | 1.00 | 13.01 | 6 | 1021 | CB  | ASP A 127 | 28.552 | 63.719 | 27.694 | 1.00 | 9.91  | 6 |
| 980  | C   | ILE A 122 | 22.464 | 51.454 | 35.289 | 1.00 | 13.96 | 6 | 1022 | CG  | ASP A 127 | 29.305 | 64.951 | 28.135 | 1.00 | 11.94 | 6 |
| 981  | O   | ILE A 122 | 22.075 | 50.945 | 34.227 | 1.00 | 12.86 | 8 | 1023 | OD1 | ASP A 127 | 28.822 | 66.041 | 27.747 | 1.00 | 11.17 | 8 |
| 982  | CB  | ILE A 122 | 24.556 | 50.129 | 35.886 | 1.00 | 12.06 | 6 | 1024 | OD2 | ASP A 127 | 30.335 | 64.880 | 28.865 | 1.00 | 10.63 | 8 |
| 983  | CG1 | ILE A 122 | 25.320 | 49.424 | 37.040 | 1.00 | 15.35 | 6 | 1025 | N   | PHE A 128 | 25.802 | 65.484 | 26.325 | 1.00 | 8.41  | 7 |
| 984  | CG2 | ILE A 122 | 25.415 | 51.348 | 35.506 | 1.00 | 13.36 | 6 | 1026 | CA  | PHE A 128 | 25.134 | 65.952 | 25.077 | 1.00 | 9.40  | 6 |
| 985  | CD1 | ILE A 122 | 26.569 | 48.709 | 36.465 | 1.00 | 15.31 | 6 | 1027 | C   | PHE A 128 | 25.609 | 67.394 | 24.887 | 1.00 | 9.48  | 6 |
| 986  | N   | LYS A 123 | 22.344 | 52.752 | 35.609 | 1.00 | 11.45 | 7 | 1028 | O   | PHE A 128 | 25.752 | 68.163 | 25.858 | 1.00 | 10.67 | 8 |
| 987  | CA  | LYS A 123 | 21.767 | 53.718 | 34.652 | 1.00 | 11.74 | 6 | 1029 | CB  | PHE A 128 | 23.609 | 66.006 | 25.437 | 1.00 | 9.59  | 6 |
| 988  | C   | LYS A 123 | 22.865 | 54.362 | 33.786 | 1.00 | 11.74 | 6 | 1030 | CG  | PHE A 128 | 22.760 | 66.405 | 24.223 | 1.00 | 8.93  | 6 |
| 989  | O   | LYS A 123 | 24.052 | 54.129 | 34.057 | 1.00 | 11.17 | 8 | 1031 | CD1 | PHE A 128 | 22.719 | 65.597 | 23.104 | 1.00 | 12.26 | 6 |
| 990  | CB  | LYS A 123 | 21.051 | 54.811 | 35.457 | 1.00 | 11.34 | 6 | 1032 | CD2 | PHE A 128 | 22.095 | 67.627 | 24.315 | 1.00 | 10.12 | 6 |
| 991  | CG  | LYS A 123 | 19.832 | 54.205 | 36.163 | 1.00 | 12.23 | 6 | 1033 | CE1 | PHE A 128 | 21.907 | 66.014 | 22.027 | 1.00 | 12.04 | 6 |
| 992  | CD  | LYS A 123 | 18.994 | 55.310 | 36.815 | 1.00 | 16.30 | 6 | 1034 | CE2 | PHE A 128 | 21.325 | 67.993 | 23.183 | 1.00 | 10.05 | 6 |
| 993  | CE  | LYS A 123 | 19.601 | 56.014 | 38.025 | 1.00 | 21.38 | 6 | 1035 | CZ  | PHE A 128 | 21.229 | 67.218 | 22.070 | 1.00 | 10.20 | 6 |
| 994  | NZ  | LYS A 123 | 20.133 | 55.054 | 39.000 | 1.00 | 25.83 | 7 | 1036 | N   | VAL A 129 | 25.985 | 67.736 | 23.647 | 1.00 | 8.13  | 7 |
| 995  | N   | VAL A 124 | 22.372 | 54.936 | 32.656 | 1.00 | 9.54  | 7 | 1037 | CA  | VAL A 129 | 26.851 | 68.932 | 23.398 | 1.00 | 9.78  | 6 |
| 996  | CA  | VAL A 124 | 23.343 | 55.533 | 31.740 | 1.00 | 9.53  | 6 | 1038 | C   | VAL A 129 | 26.171 | 69.845 | 22.412 | 1.00 | 9.18  | 6 |
| 997  | C   | VAL A 124 | 22.856 | 56.954 | 31.460 | 1.00 | 12.31 | 6 | 1039 | O   | VAL A 129 | 26.494 | 70.026 | 21.210 | 1.00 | 10.74 | 8 |
| 998  | O   | VAL A 124 | 21.723 | 57.168 | 30.990 | 1.00 | 12.23 | 8 | 1040 | CB  | VAL A 129 | 28.178 | 68.381 | 22.804 | 1.00 | 11.28 | 6 |
| 999  | CB  | VAL A 124 | 23.372 | 54.748 | 30.408 | 1.00 | 12.71 | 6 | 1041 | CG1 | VAL A 129 | 29.206 | 69.539 | 22.719 | 1.00 | 12.02 | 6 |
| 1000 | CG1 | VAL A 124 | 24.327 | 55.480 | 29.398 | 1.00 | 12.93 | 6 | 1042 | CG2 | VAL A 129 | 28.829 | 67.246 | 23.590 | 1.00 | 10.62 | 6 |
| 1001 | CG2 | VAL A 124 | 23.875 | 53.313 | 30.661 | 1.00 | 11.85 | 6 | 1043 | N   | PRO A 130 | 25.165 | 70.638 | 22.855 | 1.00 | 10.64 | 7 |
| 1002 | N   | ILE A 125 | 23.726 | 57.937 | 31.756 | 1.00 | 10.85 | 7 | 1044 | CA  | PRO A 130 | 24.341 | 71.474 | 21.986 | 1.00 | 10.69 | 6 |
| 1003 | CA  | ILE A 125 | 23.419 | 59.311 | 31.352 | 1.00 | 10.22 | 6 | 1045 | C   | PRO A 130 | 24.946 | 72.802 | 21.588 | 1.00 | 11.36 | 6 |
| 1004 | C   | ILE A 125 | 24.430 | 59.676 | 30.232 | 1.00 | 11.59 | 6 | 1046 | O   | PRO A 130 | 22.336 | 73.565 | 20.814 | 1.00 | 11.49 | 8 |
| 1005 | O   | ILE A 125 | 25.549 | 59.113 | 30.220 | 1.00 | 12.11 | 8 | 1047 | CB  | PRO A 130 | 22.983 | 71.673 | 22.735 | 1.00 | 10.77 | 6 |
| 1006 | CB  | ILE A 125 | 23.403 | 60.385 | 32.474 | 1.00 | 10.25 | 6 | 1048 | CG  | PRO A 130 | 23.480 | 71.602 | 24.189 | 1.00 | 12.02 | 6 |
| 1007 | CG1 | ILE A 125 | 24.811 | 60.531 | 33.089 | 1.00 | 13.12 | 6 | 1049 | CD  | PRO A 130 | 24.593 | 70.514 | 24.205 | 1.00 | 11.44 | 6 |
| 1008 | CG2 | ILE A 125 | 22.304 | 60.035 | 33.484 | 1.00 | 9.99  | 6 | 1050 | N   | ASN A 131 | 26.107 | 73.181 | 22.144 | 1.00 | 9.48  | 7 |
| 1009 | CD1 | ILE A 125 | 24.770 | 61.746 | 34.084 | 1.00 | 17.03 | 6 | 1051 | CA  | ASN A 131 | 26.687 | 74.481 | 21.859 | 1.00 | 10.43 | 6 |
| 1010 | N   | VAL A 126 | 23.971 | 60.450 | 29.252 | 1.00 | 9.62  | 7 | 1052 | C   | ASN A 131 | 27.244 | 74.637 | 20.438 | 1.00 | 11.66 | 6 |
| 1011 | CA  | VAL A 126 | 24.864 | 60.725 | 28.102 | 1.00 | 10.33 | 6 | 1053 | O   | ASN A 131 | 27.256 | 75.724 | 19.881 | 1.00 | 11.65 | 8 |

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|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1054 | CB  | ASN A 131 | 27.756 | 74.902 | 22.877 | 1.00 | 10.94 | 6 | 1096 | CE1 | PHE A 136 | 33.813 | 78.477 | 13.738 | 1.00 | 13.44 | 6 |
| 1055 | CG  | ASN A 131 | 28.233 | 76.316 | 22.592 | 1.00 | 10.72 | 6 | 1097 | CE2 | PHE A 136 | 34.451 | 79.741 | 11.779 | 1.00 | 12.17 | 6 |
| 1056 | OD1 | ASN A 131 | 27.396 | 77.205 | 22.783 | 1.00 | 10.02 | 8 | 1098 | CZ  | PHE A 136 | 33.903 | 79.708 | 13.087 | 1.00 | 15.41 | 6 |
| 1057 | ND2 | ASN A 131 | 29.516 | 76.447 | 22.224 | 1.00 | 10.08 | 7 | 1099 | N   | LYS A 137 | 38.037 | 77.258 | 10.547 | 1.00 | 11.70 | 7 |
| 1058 | N   | HIS A 132 | 27.676 | 73.513 | 19.855 | 1.00 | 10.71 | 7 | 1100 | CA  | LYS A 137 | 38.710 | 78.567 | 10.479 | 1.00 | 10.33 | 6 |
| 1059 | CA  | HIS A 132 | 28.476 | 73.726 | 18.632 | 1.00 | 9.32  | 6 | 1101 | C   | LYS A 137 | 37.859 | 79.484 | 9.618  | 1.00 | 13.10 | 6 |
| 1060 | C   | HIS A 132 | 28.552 | 72.441 | 17.845 | 1.00 | 9.83  | 6 | 1102 | O   | LYS A 137 | 37.493 | 79.111 | 8.490  | 1.00 | 12.91 | 8 |
| 1061 | O   | HIS A 132 | 28.256 | 71.362 | 18.361 | 1.00 | 12.46 | 8 | 1103 | CB  | LYS A 137 | 40.060 | 78.360 | 9.724  | 1.00 | 17.76 | 6 |
| 1062 | CB  | HIS A 132 | 29.896 | 74.227 | 19.005 | 1.00 | 11.52 | 6 | 1104 | CG  | LYS A 137 | 41.153 | 77.554 | 10.411 | 1.00 | 19.69 | 6 |
| 1063 | CG  | HIS A 132 | 30.560 | 73.394 | 20.080 | 1.00 | 10.70 | 6 | 1105 | CD  | LYS A 137 | 41.439 | 78.049 | 11.810 | 1.00 | 22.72 | 6 |
| 1064 | ND1 | HIS A 132 | 30.616 | 73.869 | 21.372 | 1.00 | 11.00 | 7 | 1106 | CE  | LYS A 137 | 42.145 | 79.366 | 12.006 | 1.00 | 31.41 | 6 |
| 1065 | CD2 | HIS A 132 | 31.084 | 72.152 | 20.032 | 1.00 | 9.99  | 6 | 1107 | NZ  | LYS A 137 | 43.212 | 79.771 | 11.035 | 1.00 | 25.39 | 7 |
| 1066 | CE1 | HIS A 132 | 31.189 | 72.945 | 22.154 | 1.00 | 12.39 | 6 | 1108 | N   | ALA A 138 | 37.657 | 80.688 | 10.158 | 1.00 | 12.09 | 7 |
| 1067 | NE2 | HIS A 132 | 31.445 | 71.929 | 21.368 | 1.00 | 10.00 | 7 | 1109 | CA  | ALA A 138 | 36.683 | 81.510 | 9.375  | 1.00 | 12.57 | 6 |
| 1068 | N   | SER A 133 | 28.999 | 72.608 | 16.584 | 1.00 | 10.23 | 7 | 1110 | C   | ALA A 138 | 37.267 | 81.873 | 8.017  | 1.00 | 14.60 | 6 |
| 1069 | CA  | SER A 133 | 29.365 | 71.428 | 15.787 | 1.00 | 10.30 | 6 | 1111 | O   | ALA A 138 | 36.410 | 82.176 | 7.094  | 1.00 | 14.01 | 8 |
| 1070 | C   | SER A 133 | 30.876 | 71.239 | 15.861 | 1.00 | 11.64 | 6 | 1112 | CB  | ALA A 138 | 36.469 | 82.806 | 10.148 | 1.00 | 15.45 | 6 |
| 1071 | O   | SER A 133 | 31.319 | 70.652 | 16.863 | 1.00 | 11.94 | 8 | 1113 | N   | ASN A 139 | 38.597 | 81.986 | 7.900  | 1.00 | 13.25 | 7 |
| 1072 | CB  | SER A 133 | 28.807 | 71.514 | 14.344 | 1.00 | 10.65 | 6 | 1114 | CA  | ASN A 139 | 39.165 | 82.359 | 6.608  | 1.00 | 14.41 | 6 |
| 1073 | OG  | SER A 133 | 29.342 | 72.683 | 13.700 | 1.00 | 11.57 | 8 | 1115 | C   | ASN A 139 | 39.444 | 81.212 | 5.682  | 1.00 | 14.25 | 6 |
| 1074 | N   | THR A 134 | 31.611 | 71.535 | 14.805 | 1.00 | 11.30 | 7 | 1116 | O   | ASN A 139 | 40.047 | 81.349 | 4.562  | 1.00 | 14.82 | 8 |
| 1075 | CA  | THR A 134 | 33.034 | 71.082 | 14.740 | 1.00 | 10.51 | 6 | 1117 | CB  | ASN A 139 | 40.443 | 83.188 | 6.852  | 1.00 | 16.78 | 6 |
| 1076 | C   | THR A 134 | 33.959 | 72.251 | 14.424 | 1.00 | 8.56  | 6 | 1118 | CG  | ASN A 139 | 41.666 | 82.292 | 7.083  | 1.00 | 22.27 | 6 |
| 1077 | O   | THR A 134 | 33.553 | 73.376 | 14.121 | 1.00 | 10.40 | 8 | 1119 | OD1 | ASN A 139 | 41.484 | 81.167 | 7.486  | 1.00 | 25.66 | 8 |
| 1078 | CB  | THR A 134 | 33.119 | 70.005 | 13.630 | 1.00 | 9.65  | 6 | 1120 | ND2 | ASN A 139 | 42.853 | 82.762 | 6.773  | 1.00 | 21.53 | 7 |
| 1079 | OG1 | THR A 134 | 32.559 | 70.596 | 12.429 | 1.00 | 11.51 | 8 | 1121 | N   | ASP A 140 | 39.150 | 79.955 | 6.052  | 1.00 | 14.76 | 7 |
| 1080 | CG2 | THR A 134 | 32.295 | 68.752 | 13.956 | 1.00 | 11.00 | 6 | 1122 | CA  | ASP A 140 | 39.433 | 78.835 | 5.203  | 1.00 | 13.60 | 6 |
| 1081 | N   | PRO A 135 | 35.256 | 71.959 | 14.489 | 1.00 | 10.51 | 7 | 1123 | C   | ASP A 140 | 38.470 | 77.674 | 5.337  | 1.00 | 16.09 | 6 |
| 1082 | CA  | PRO A 135 | 36.320 | 72.955 | 14.289 | 1.00 | 12.33 | 6 | 1124 | O   | ASP A 140 | 38.607 | 76.905 | 6.339  | 1.00 | 13.95 | 8 |
| 1083 | C   | PRO A 135 | 36.264 | 73.606 | 12.899 | 1.00 | 12.27 | 6 | 1125 | CB  | ASP A 140 | 40.885 | 78.382 | 5.557  | 1.00 | 12.14 | 6 |
| 1084 | O   | PRO A 135 | 36.014 | 72.968 | 11.868 | 1.00 | 13.19 | 8 | 1126 | CG  | ASP A 140 | 41.331 | 77.260 | 4.643  | 1.00 | 16.87 | 6 |
| 1085 | CB  | PRO A 135 | 37.627 | 72.145 | 14.405 | 1.00 | 11.11 | 6 | 1127 | OD1 | ASP A 140 | 40.616 | 76.705 | 3.810  | 1.00 | 17.82 | 8 |
| 1086 | CG  | PRO A 135 | 37.241 | 71.129 | 15.486 | 1.00 | 11.56 | 6 | 1128 | OD2 | ASP A 140 | 42.569 | 76.954 | 4.814  | 1.00 | 25.09 | 8 |
| 1087 | CD  | PRO A 135 | 35.809 | 70.746 | 15.111 | 1.00 | 11.98 | 6 | 1129 | N   | SER A 141 | 37.529 | 77.555 | 4.414  | 1.00 | 15.21 | 7 |
| 1088 | N   | PHE A 136 | 36.500 | 74.966 | 12.885 | 1.00 | 10.88 | 7 | 1130 | CA  | SER A 141 | 36.508 | 76.520 | 4.501  | 1.00 | 16.63 | 6 |
| 1089 | CA  | PHE A 136 | 36.606 | 75.628 | 11.597 | 1.00 | 11.37 | 6 | 1131 | C   | SER A 141 | 37.048 | 75.092 | 4.285  | 1.00 | 17.44 | 6 |
| 1090 | C   | PHE A 136 | 37.536 | 76.830 | 11.718 | 1.00 | 11.99 | 6 | 1132 | O   | SER A 141 | 36.349 | 74.129 | 4.607  | 1.00 | 18.28 | 8 |
| 1091 | O   | PHE A 136 | 37.856 | 77.248 | 12.827 | 1.00 | 12.95 | 8 | 1133 | CB  | SER A 141 | 35.372 | 76.746 | 3.493  | 1.00 | 19.52 | 6 |
| 1092 | CB  | PHE A 136 | 35.176 | 76.074 | 11.125 | 1.00 | 13.36 | 6 | 1134 | OG  | SER A 141 | 35.867 | 76.579 | 2.144  | 1.00 | 16.38 | 8 |
| 1093 | CG  | PHE A 136 | 34.690 | 77.341 | 11.793 | 1.00 | 15.31 | 6 | 1135 | N   | THR A 142 | 38.302 | 74.958 | 3.839  | 1.00 | 14.08 | 7 |
| 1094 | CD1 | PHE A 136 | 34.201 | 77.311 | 13.100 | 1.00 | 12.18 | 6 | 1136 | CA  | THR A 142 | 38.889 | 73.615 | 3.649  | 1.00 | 15.63 | 6 |
| 1095 | CD2 | PHE A 136 | 34.801 | 78.565 | 11.134 | 1.00 | 13.24 | 6 | 1137 | C   | THR A 142 | 39.445 | 73.036 | 4.933  | 1.00 | 16.91 | 6 |



|      |     |           |        |        |        |      |       |    |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1222 | C   | THR A 154 | 22.181 | 65.781 | 5.538  | 1.00 | 14.24 | 6  | 1264 | CG  | TYR A 159 | 31.171 | 79.475 | 10.063 | 1.00 | 11.61 | 6 |
| 1223 | O   | THR A 154 | 22.048 | 66.264 | 6.650  | 1.00 | 15.31 | 8  | 1265 | CD1 | TYR A 159 | 30.414 | 79.868 | 11.149 | 1.00 | 14.86 | 6 |
| 1224 | CB  | THR A 154 | 20.008 | 64.592 | 5.212  | 1.00 | 21.10 | 6  | 1266 | CD2 | TYR A 159 | 31.962 | 80.402 | 9.380  | 1.00 | 13.87 | 6 |
| 1225 | OG1 | THR A 154 | 19.488 | 63.334 | 4.709  | 1.00 | 20.66 | 8  | 1267 | CE1 | TYR A 159 | 30.576 | 81.181 | 11.600 | 1.00 | 15.19 | 6 |
| 1226 | OG2 | THR A 154 | 19.569 | 65.711 | 4.260  | 1.00 | 21.99 | 6  | 1268 | CE2 | TYR A 159 | 32.069 | 81.716 | 9.811  | 1.00 | 19.88 | 6 |
| 1227 | N   | TYR A 155 | 22.977 | 66.280 | 4.566  | 1.00 | 14.57 | 7  | 1269 | CZ  | TYR A 159 | 31.387 | 82.088 | 10.926 | 1.00 | 16.15 | 6 |
| 1228 | CA  | TYR A 155 | 23.613 | 67.573 | 4.928  | 1.00 | 15.65 | 6  | 1270 | OH  | TYR A 159 | 31.377 | 83.383 | 11.432 | 1.00 | 16.24 | 8 |
| 1229 | C   | TYR A 155 | 22.652 | 68.698 | 5.184  | 1.00 | 17.55 | 6  | 1271 | N   | PHE A 160 | 29.904 | 78.307 | 6.253  | 1.00 | 13.52 | 7 |
| 1230 | O   | TYR A 155 | 21.639 | 68.912 | 4.487  | 1.00 | 16.44 | 8  | 1272 | CA  | PHE A 160 | 30.073 | 79.126 | 5.029  | 1.00 | 12.84 | 6 |
| 1231 | CB  | TYR A 155 | 24.440 | 67.984 | 3.678  | 1.00 | 16.08 | 6  | 1273 | C   | PHE A 160 | 28.855 | 79.182 | 4.153  | 1.00 | 12.34 | 6 |
| 1232 | CG  | TYR A 155 | 25.238 | 69.243 | 3.820  | 1.00 | 16.71 | 6  | 1274 | O   | PHE A 160 | 28.803 | 80.101 | 3.300  | 1.00 | 14.63 | 8 |
| 1233 | CD1 | TYR A 155 | 26.324 | 69.277 | 4.693  | 1.00 | 16.20 | 6  | 1275 | CB  | PHE A 160 | 31.228 | 78.421 | 4.234  | 1.00 | 12.99 | 6 |
| 1234 | CD2 | TYR A 155 | 24.989 | 70.381 | 3.075  | 1.00 | 16.54 | 6  | 1276 | CG  | PHE A 160 | 32.504 | 78.508 | 5.080  | 1.00 | 14.21 | 6 |
| 1235 | CE1 | TYR A 155 | 27.139 | 70.407 | 4.789  | 1.00 | 16.44 | 6  | 1277 | CD1 | PHE A 160 | 33.310 | 79.662 | 4.935  | 1.00 | 12.64 | 6 |
| 1236 | CE2 | TYR A 155 | 25.773 | 71.530 | 3.162  | 1.00 | 14.17 | 6  | 1278 | CD2 | PHE A 160 | 32.804 | 77.488 | 5.965  | 1.00 | 12.84 | 6 |
| 1237 | CZ  | TYR A 155 | 26.843 | 71.515 | 4.015  | 1.00 | 16.83 | 6  | 1279 | CE1 | PHE A 160 | 34.466 | 79.772 | 5.737  | 1.00 | 14.91 | 6 |
| 1238 | OH  | TYR A 155 | 27.673 | 72.601 | 4.142  | 1.00 | 15.80 | 8  | 1280 | CE2 | PHE A 160 | 33.940 | 77.621 | 6.761  | 1.00 | 14.27 | 6 |
| 1239 | N   | MET A 156 | 22.895 | 69.456 | 6.272  | 1.00 | 12.36 | 7  | 1281 | CZ  | PHE A 160 | 34.769 | 78.740 | 6.653  | 1.00 | 13.93 | 6 |
| 1240 | CA  | MET A 156 | 22.120 | 70.658 | 6.595  | 1.00 | 12.72 | 6  | 1282 | N   | ASP A 161 | 27.917 | 78.220 | 4.232  | 1.00 | 14.16 | 7 |
| 1241 | C   | MET A 156 | 22.877 | 71.939 | 6.202  | 1.00 | 14.70 | 6  | 1283 | CA  | ASP A 161 | 26.731 | 78.329 | 3.371  | 1.00 | 14.46 | 6 |
| 1242 | O   | MET A 156 | 22.290 | 72.876 | 5.628  | 1.00 | 14.86 | 8  | 1284 | C   | ASP A 161 | 25.486 | 78.622 | 4.217  | 1.00 | 14.25 | 6 |
| 1243 | CB  | MET A 156 | 21.886 | 70.683 | 8.141  | 1.00 | 14.72 | 6  | 1285 | O   | ASP A 161 | 24.375 | 78.215 | 3.808  | 1.00 | 15.23 | 8 |
| 1244 | CG  | MET A 156 | 21.045 | 69.510 | 8.543  | 1.00 | 13.16 | 6  | 1286 | CB  | ASP A 161 | 26.557 | 77.031 | 2.565  | 1.00 | 12.66 | 6 |
| 1245 | SD  | MET A 156 | 20.812 | 69.391 | 10.354 | 1.00 | 16.44 | 16 | 1287 | CG  | ASP A 161 | 26.500 | 75.766 | 3.373  | 1.00 | 15.7  |   |



|      |     |     |   |     |        |        |        |      |       |   |      |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 1306 | O   | THR | A | 164 | 18.055 | 80.605 | 5.002  | 1.00 | 25.38 | 8 | 1348 | C   | HIS | A | 169 | 27.266 | 82.836 | 14.195 | 1.00 | 11.69 | 6 |
| 1307 | CB  | THR | A | 164 | 19.384 | 81.502 | 2.723  | 1.00 | 21.33 | 6 | 1349 | O   | HIS | A | 169 | 28.109 | 82.035 | 13.921 | 1.00 | 11.66 | 8 |
| 1308 | OG1 | THR | A | 164 | 19.834 | 80.146 | 2.496  | 1.00 | 29.22 | 8 | 1350 | CB  | HIS | A | 169 | 26.361 | 82.658 | 16.482 | 1.00 | 11.57 | 6 |
| 1309 | CG2 | THR | A | 164 | 20.062 | 82.359 | 1.658  | 1.00 | 32.67 | 6 | 1351 | CG  | HIS | A | 169 | 25.157 | 82.347 | 17.376 | 1.00 | 11.97 | 6 |
| 1310 | N   | LYS | A | 165 | 20.086 | 80.431 | 6.008  | 1.00 | 19.16 | 7 | 1352 | ND1 | HIS | A | 169 | 25.403 | 81.657 | 18.588 | 1.00 | 11.36 | 7 |
| 1311 | CA  | LYS | A | 165 | 19.577 | 79.430 | 6.929  | 1.00 | 16.62 | 6 | 1353 | CD2 | HIS | A | 169 | 23.838 | 82.604 | 17.274 | 1.00 | 11.55 | 6 |
| 1312 | C   | LYS | A | 165 | 19.714 | 79.888 | 8.391  | 1.00 | 18.03 | 6 | 1354 | CE1 | HIS | A | 169 | 24.195 | 81.518 | 19.195 | 1.00 | 12.02 | 6 |
| 1313 | O   | LYS | A | 165 | 18.735 | 79.767 | 9.173  | 1.00 | 17.25 | 8 | 1355 | NE2 | HIS | A | 169 | 23.233 | 82.111 | 18.427 | 1.00 | 10.80 | 7 |
| 1314 | CB  | LYS | A | 165 | 20.423 | 78.140 | 6.826  | 1.00 | 13.80 | 6 | 1356 | N   | HIS | A | 170 | 27.295 | 84.147 | 13.797 | 1.00 | 11.77 | 7 |
| 1315 | CG  | LYS | A | 165 | 20.215 | 77.497 | 5.423  | 1.00 | 21.49 | 6 | 1357 | CA  | HIS | A | 170 | 28.474 | 84.629 | 13.015 | 1.00 | 12.20 | 6 |
| 1316 | CD  | LYS | A | 165 | 20.913 | 76.186 | 5.334  | 1.00 | 30.47 | 6 | 1358 | C   | HIS | A | 170 | 29.029 | 85.872 | 13.672 | 1.00 | 14.93 | 6 |
| 1317 | CE  | LYS | A | 165 | 22.394 | 76.297 | 5.245  | 1.00 | 26.09 | 6 | 1359 | O   | HIS | A | 170 | 29.174 | 86.974 | 13.053 | 1.00 | 16.92 | 8 |
| 1318 | NZ  | LYS | A | 165 | 23.067 | 75.308 | 4.349  | 1.00 | 18.44 | 7 | 1360 | CB  | HIS | A | 170 | 28.083 | 84.949 | 11.533 | 1.00 | 13.28 | 6 |
| 1319 | N   | GLY | A | 166 | 20.839 | 80.499 | 8.700  | 1.00 | 14.27 | 7 | 1361 | CG  | HIS | A | 170 | 27.535 | 83.698 | 10.888 | 1.00 | 12.02 | 6 |
| 1320 | CA  | GLY | A | 166 | 21.048 | 81.024 | 10.082 | 1.00 | 14.43 | 6 | 1362 | ND1 | HIS | A | 170 | 28.327 | 82.925 | 10.069 | 1.00 | 15.51 | 7 |
| 1321 | C   | GLY | A | 166 | 21.103 | 79.863 | 11.109 | 1.00 | 14.80 | 6 | 1363 | CD2 | HIS | A | 170 | 26.306 | 83.088 | 10.915 | 1.00 | 13.12 | 6 |
| 1322 | O   | GLY | A | 166 | 20.730 | 80.096 | 12.287 | 1.00 | 14.92 | 8 | 1364 | CE1 | HIS | A | 170 | 26.639 | 81.863 | 9.689  | 1.00 | 16.69 | 6 |
| 1323 | N   | TYR | A | 167 | 21.732 | 78.765 | 10.734 | 1.00 | 12.78 | 7 | 1365 | NE2 | HIS | A | 170 | 26.409 | 81.953 | 10.156 | 1.00 | 13.32 | 7 |
| 1324 | CA  | TYR | A | 167 | 21.882 | 77.692 | 11.732 | 1.00 | 12.54 | 6 | 1366 | N   | ASN | A | 171 | 29.387 | 85.778 | 14.962 | 1.00 | 12.58 | 7 |
| 1325 | C   | TYR | A | 167 | 22.991 | 78.009 | 12.739 | 1.00 | 12.62 | 6 | 1367 | CA  | ASN | A | 171 | 29.735 | 86.967 | 15.733 | 1.00 | 12.76 | 6 |
| 1326 | O   | TYR | A | 167 | 23.085 | 77.349 | 13.776 | 1.00 | 11.78 | 8 | 1368 | C   | ASN | A | 171 | 31.201 | 87.040 | 16.147 | 1.00 | 13.34 | 6 |
| 1327 | CB  | TYR | A | 167 | 22.226 | 76.374 | 11.022 | 1.00 | 10.92 | 6 | 1369 | O   | ASN | A | 171 | 31.554 | 87.947 | 16.949 | 1.00 | 17.31 | 8 |
| 1328 | CG  | TYR | A | 167 | 21.127 | 75.836 | 10.103 | 1.00 | 14.63 | 6 | 1370 | CB  | ASN | A | 171 | 28.916 | 86.961 | 17.054 | 1.00 | 13.40 | 6 |
| 1329 | CD1 | TYR | A | 167 | 19.810 | 76.232 | 10.291 | 1.00 | 13.59 | 6 | 1371 | CG  | ASN | A | 171 | 27.430 | 86.948 | 16.719 | 1.00 | 17.12 | 6 |
| 1330 | CD2 | TYR | A | 167 | 21.490 | 74.921 | 9.121  | 1.00 | 15.06 | 6 | 1372 | OD1 | ASN | A | 171 | 26.595 | 86.168 | 17.252 | 1.00 | 16.54 | 8 |
| 1331 | CE1 | TYR | A | 167 | 18.836 | 75.722 | 9.421  | 1.00 | 13.53 | 6 | 1373 | ND2 | ASN | A | 171 | 27.046 | 87.866 | 15.861 | 1.00 | 12.82 | 7 |
| 1332 | CE2 | TYR | A | 167 | 20.503 | 74.385 | 8.254  | 1.00 | 12.93 | 6 | 1374 | N   | GLY | A | 172 | 32.013 | 86.197 | 15.601 | 1.00 | 13.14 | 7 |
| 1333 | CZ  | TYR | A | 167 | 19.211 | 74.809 | 8.469  | 1.00 | 15.10 | 6 | 1375 | CA  | GLY | A | 172 | 33.444 | 86.166 | 15.964 | 1.00 | 15.42 | 6 |
| 1334 | OH  | TYR | A | 167 | 18.235 | 74.289 | 7.594  | 1.00 | 18.52 | 8 | 1376 | C   | GLY | A | 172 | 33.728 | 85.275 | 17.210 | 1.00 | 16.69 | 6 |
| 1335 | N   | PHE | A | 168 | 23.963 | 78.870 | 12.342 | 1.00 | 11.36 | 7 | 1377 | O   | GLY | A | 172 | 32.817 | 84.706 | 17.722 | 1.00 | 14.98 | 8 |
| 1336 | CA  | PHE | A | 168 | 25.072 | 79.208 | 13.244 | 1.00 | 11.20 | 6 | 1378 | N   | ASP | A | 173 | 34.993 | 85.180 | 17.526 | 1.00 | 14.76 | 7 |
| 1337 | C   | PHE | A | 168 | 25.097 | 80.677 | 13.551 | 1.00 | 12.02 | 6 | 1379 | CA  | ASP | A | 173 | 35.473 | 84.346 | 18.622 | 1.00 | 12.93 | 6 |
| 1338 | O   | PHE | A | 168 | 24.515 | 81.539 | 12.854 | 1.00 | 11.21 | 8 | 1380 | C   | ASP | A | 173 | 35.292 | 84.996 | 19.976 | 1.00 | 12.76 | 6 |
| 1339 | CB  | PHE | A | 168 | 26.432 | 78.934 | 12.493 | 1.00 | 13.41 | 6 | 1381 | O   | ASP | A | 173 | 35.410 | 86.248 | 20.131 | 1.00 | 11.79 | 8 |
| 1340 | CG  | PHE | A | 168 | 26.552 | 77.459 | 12.174 | 1.00 | 11.52 | 6 | 1382 | CB  | ASP | A | 173 | 36.980 | 84.152 | 18.369 | 1.00 | 14.28 | 6 |
| 1341 | CD1 | PHE | A | 168 | 27.044 | 76.583 | 13.130 | 1.00 | 10.63 | 6 | 1383 | CG  | ASP | A | 173 | 37.273 | 83.139 | 17.268 | 1.00 | 24.98 | 6 |
| 1342 | CD2 | PHE | A | 168 | 26.171 | 77.007 | 10.899 | 1.00 | 13.81 | 6 | 1384 | OD1 | ASP | A | 173 | 36.398 | 82.387 | 16.822 | 1.00 | 17.11 | 8 |
| 1343 | CE1 | PHE | A | 168 | 27.122 | 75.214 | 12.765 | 1.00 | 12.04 | 6 | 1385 | OD2 | ASP | A | 173 | 38.451 | 83.124 | 16.815 | 1.00 | 23.71 | 8 |
| 1344 | CE2 | PHE | A | 168 | 26.250 | 75.639 | 10.574 | 1.00 | 12.05 | 6 | 1386 | N   | ILE | A | 174 | 35.073 | 84.127 | 20.969 | 1.00 | 12.58 | 7 |
| 1345 | CZ  | PHE | A | 168 | 26.752 | 74.751 | 11.518 | 1.00 | 12.13 | 6 | 1387 | CA  | ILE | A | 174 | 35.136 | 84.670 | 22.362 | 1.00 | 11.65 | 6 |
| 1346 | N   | HIS | A | 169 | 25.665 | 81.067 | 14.709 | 1.00 | 11.43 | 7 | 1388 | C   | ILE | A | 174 | 36.500 | 85.307 | 22.646 | 1.00 | 14.87 | 6 |
| 1347 | CA  | HIS | A | 169 | 25.979 | 82.473 | 14.979 | 1.00 | 12.52 | 6 | 1389 | O   | ILE | A | 174 | 37.508 | 84.670 | 22.337 | 1.00 | 15.09 | 8 |

|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1390 | CB  | ILE A 174 | 34.896 | 83.495 | 23.357 | 1.00 | 13.27 | 6 | 1432 | C   | ASP A 179 | 30.292 | 87.603 | 28.903 | 1.00 | 12.33 | 6 |
| 1391 | CG1 | ILE A 174 | 33.431 | 83.005 | 23.177 | 1.00 | 10.95 | 6 | 1433 | O   | ASP A 179 | 30.537 | 86.725 | 28.067 | 1.00 | 12.08 | 8 |
| 1392 | CG2 | ILE A 174 | 35.145 | 84.016 | 24.806 | 1.00 | 12.74 | 6 | 1434 | CB  | ASP A 179 | 31.997 | 89.341 | 28.184 | 1.00 | 15.43 | 6 |
| 1393 | CD1 | ILE A 174 | 33.220 | 81.690 | 24.000 | 1.00 | 11.77 | 6 | 1435 | CG  | ASP A 179 | 30.831 | 90.225 | 27.763 | 1.00 | 18.80 | 6 |
| 1394 | N   | SER A 175 | 36.441 | 86.493 | 23.260 | 1.00 | 14.22 | 7 | 1436 | OD1 | ASP A 179 | 30.462 | 91.232 | 28.431 | 1.00 | 20.56 | 8 |
| 1395 | CA  | SER A 175 | 37.710 | 87.093 | 23.770 | 1.00 | 16.89 | 6 | 1437 | OD2 | ASP A 179 | 30.213 | 89.893 | 26.753 | 1.00 | 13.51 | 8 |
| 1396 | C   | SER A 175 | 37.712 | 87.131 | 25.291 | 1.00 | 18.02 | 6 | 1438 | N   | ARG A 180 | 29.115 | 87.768 | 29.477 | 1.00 | 13.02 | 7 |
| 1397 | O   | SER A 175 | 38.617 | 86.587 | 25.938 | 1.00 | 19.20 | 8 | 1439 | CA  | ARG A 180 | 28.057 | 86.771 | 29.205 | 1.00 | 11.54 | 6 |
| 1398 | CB  | SER A 175 | 37.868 | 88.470 | 23.138 | 1.00 | 17.86 | 6 | 1440 | C   | ARG A 180 | 27.585 | 86.833 | 27.757 | 1.00 | 10.36 | 6 |
| 1399 | OG  | SER A 175 | 39.049 | 89.044 | 23.724 | 1.00 | 24.28 | 8 | 1441 | O   | ARG A 180 | 27.261 | 85.746 | 27.225 | 1.00 | 11.27 | 8 |
| 1400 | N   | ASN A 176 | 36.650 | 87.662 | 25.854 | 1.00 | 14.39 | 7 | 1442 | CB  | ARG A 180 | 26.893 | 87.051 | 30.172 | 1.00 | 13.31 | 6 |
| 1401 | CA  | ASN A 176 | 36.515 | 87.678 | 27.336 | 1.00 | 13.41 | 6 | 1443 | CG  | ARG A 180 | 27.286 | 86.796 | 31.654 | 1.00 | 12.49 | 6 |
| 1402 | C   | ASN A 176 | 35.511 | 86.561 | 27.678 | 1.00 | 12.76 | 6 | 1444 | CD  | ARG A 180 | 27.797 | 85.340 | 31.899 | 1.00 | 10.75 | 6 |
| 1403 | O   | ASN A 176 | 34.286 | 86.760 | 27.482 | 1.00 | 13.43 | 8 | 1445 | NE  | ARG A 180 | 26.694 | 84.389 | 31.571 | 1.00 | 11.38 | 7 |
| 1404 | CB  | ASN A 176 | 35.898 | 89.032 | 27.724 | 1.00 | 15.61 | 6 | 1446 | CZ  | ARG A 180 | 26.896 | 83.305 | 30.812 | 1.00 | 11.55 | 6 |
| 1405 | CG  | ASN A 176 | 35.749 | 89.123 | 29.243 | 1.00 | 17.91 | 6 | 1447 | NH1 | ARG A 180 | 28.090 | 82.893 | 30.359 | 1.00 | 11.21 | 7 |
| 1406 | OD1 | ASN A 176 | 35.963 | 88.166 | 29.982 | 1.00 | 15.18 | 8 | 1448 | NH2 | ARG A 180 | 25.769 | 82.597 | 30.589 | 1.00 | 13.64 | 7 |
| 1407 | ND2 | ASN A 176 | 35.402 | 90.347 | 29.694 | 1.00 | 22.13 | 7 | 1449 | N   | TYR A 181 | 27.508 | 87.990 | 27.113 | 1.00 | 10.51 | 7 |
| 1408 | N   | TRP A 177 | 36.085 | 85.465 | 28.237 | 1.00 | 14.29 | 7 | 1450 | CA  | TYR A 181 | 27.104 | 87.980 | 25.688 | 1.00 | 10.68 | 6 |
| 1409 | CA  | TRP A 177 | 35.172 | 84.361 | 28.558 | 1.00 | 13.39 | 6 | 1451 | C   | TYR A 181 | 28.195 | 87.277 | 24.870 | 1.00 | 11.14 | 6 |
| 1410 | C   | TRP A 177 | 34.248 | 84.677 | 29.724 | 1.00 | 15.05 | 6 | 1452 | O   | TYR A 181 | 27.826 | 86.403 | 24.044 | 1.00 | 10.66 | 8 |
| 1411 | O   | TRP A 177 | 33.279 | 83.898 | 29.909 | 1.00 | 14.25 | 8 | 1453 | CB  | TYR A 181 | 26.915 | 89.446 | 25.196 | 1.00 | 12.30 | 6 |
| 1412 | CB  | TRP A 177 | 36.054 | 83.145 | 28.953 | 1.00 | 16.12 | 6 | 1454 | CG  | TYR A 181 | 26.645 | 89.417 | 23.698 | 1.00 | 12.16 | 6 |
| 1413 | CG  | TRP A 177 | 36.712 | 82.559 | 27.721 | 1.00 | 14.43 | 6 | 1455 | CD1 | TYR A 181 | 25.446 | 89.009 | 23.179 | 1.00 | 13.07 | 6 |
| 1414 | CD1 | TRP A 177 | 37.745 | 83.101 | 26.998 | 1.00 | 16.58 | 6 | 1456 | CD2 | TYR A 181 | 27.712 | 89.736 | 22.837 | 1.00 | 15.09 | 6 |
| 1415 | CD2 | TRP A 177 | 36.399 | 81.291 | 27.142 | 1.00 | 13.92 | 6 | 1457 | CE1 | TYR A 181 | 25.242 | 88.936 | 21.808 | 1.00 | 18.03 | 6 |
| 1416 | NE1 | TRP A 177 | 38.070 | 82.235 | 25.940 | 1.00 | 18.57 | 7 | 1458 | CE2 | TYR A 181 | 27.510 | 89.688 | 21.457 | 1.00 | 16.90 | 6 |
| 1417 | CE2 | TRP A 177 | 37.234 | 81.131 | 26.014 | 1.00 | 18.68 | 6 | 1459 | CZ  | TYR A 181 | 26.275 | 89.265 | 20.988 | 1.00 | 19.76 | 6 |
| 1418 | CE3 | TRP A 177 | 35.437 | 80.298 | 27.392 | 1.00 | 17.34 | 6 | 1460 | OH  | TYR A 181 | 26.097 | 89.156 | 19.614 | 1.00 | 17.30 | 8 |
| 1419 | CZ2 | TRP A 177 | 37.148 | 80.031 | 25.169 | 1.00 | 14.28 | 6 | 1461 | N   | GLU A 182 | 29.473 | 87.528 | 25.083 | 1.00 | 13.50 | 7 |
| 1420 | CZ3 | TRP A 177 | 35.379 | 79.182 | 26.574 | 1.00 | 17.20 | 6 | 1462 | CA  | GLU A 182 | 30.468 | 86.836 | 24.265 | 1.00 | 12.35 | 6 |
| 1421 | CH2 | TRP A 177 | 36.253 | 79.045 | 25.441 | 1.00 | 18.00 | 6 | 1463 | C   | GLU A 182 | 30.442 | 85.311 | 24.504 | 1.00 | 10.45 | 6 |
| 1422 | N   | ASP A 178 | 34.477 | 85.795 | 30.469 | 1.00 | 12.43 | 7 | 1464 | O   | GLU A 182 | 30.482 | 84.533 | 23.582 | 1.00 | 11.45 | 8 |
| 1423 | CA  | ASP A 178 | 33.507 | 86.126 | 31.517 | 1.00 | 11.08 | 6 | 1465 | CB  | GLU A 182 | 31.939 | 87.266 | 24.571 | 1.00 | 10.48 | 6 |
| 1424 | C   | ASP A 178 | 32.454 | 87.115 | 31.053 | 1.00 | 12.88 | 6 | 1466 | CG  | GLU A 182 | 32.131 | 88.769 | 24.214 | 1.00 | 12.66 | 6 |
| 1425 | O   | ASP A 178 | 31.586 | 87.420 | 31.881 | 1.00 | 15.73 | 8 | 1467 | CD  | GLU A 182 | 33.640 | 89.046 | 24.246 | 1.00 | 19.30 | 6 |
| 1426 | CB  | ASP A 178 | 34.243 | 86.717 | 32.739 | 1.00 | 17.78 | 6 | 1468 | OE1 | GLU A 182 | 34.487 | 88.229 | 23.958 | 1.00 | 15.48 | 8 |
| 1427 | CG  | ASP A 178 | 35.201 | 85.739 | 33.362 | 1.00 | 24.33 | 6 | 1469 | OE2 | GLU A 182 | 34.009 | 90.199 | 24.690 | 1.00 | 30.95 | 8 |
| 1428 | OD1 | ASP A 178 | 34.916 | 84.535 | 33.440 | 1.00 | 18.07 | 8 | 1470 | N   | ALA A 183 | 30.314 | 84.945 | 25.796 | 1.00 | 10.17 | 7 |
| 1429 | OD2 | ASP A 178 | 36.317 | 86.155 | 33.777 | 1.00 | 24.77 | 8 | 1471 | CA  | ALA A 183 | 30.436 | 83.521 | 26.110 | 1.00 | 11.02 | 6 |
| 1430 | N   | ASP A 179 | 32.527 | 87.608 | 29.810 | 1.00 | 11.79 | 7 | 1472 | C   | ALA A 183 | 29.302 | 82.709 | 25.471 | 1.00 | 11.67 | 6 |
| 1431 | CA  | ASP A 179 | 31.448 | 88.502 | 29.357 | 1.00 | 11.42 | 6 | 1473 | O   | ALA A 183 | 29.555 | 81.542 | 25.197 | 1.00 | 10.91 | 8 |



1558 CA PHE A 194 40.612 76.976 15.567 1.00 11.84 6 1600 CG LEU A 199 25.178 74.135 16.526 1.00 10.88 6  
1559 C PHE A 194 39.441 77.265 16.536 1.00 11.03 6 1601 CD1 LEU A 199 24.799 72.879 17.321 1.00 12.59 6  
1560 O PHE A 194 39.621 77.423 17.750 1.00 11.69 8 1602 CD2 LEU A 199 24.658 74.045 15.071 1.00 14.19 6  
1561 CB PHE A 194 40.411 75.629 14.855 1.00 10.98 6 1603 N SER A 200 23.024 78.144 16.505 1.00 11.57 7  
1562 CG PHE A 194 40.568 74.412 15.767 1.00 11.46 6 1604 CA SER A 200 22.055 79.160 16.950 1.00 10.26 6  
1563 CD1 PHE A 194 39.545 74.063 16.649 1.00 11.56 6 1605 C SER A 200 20.810 78.424 17.499 1.00 11.50 6  
1564 CD2 PHE A 194 41.707 73.656 15.747 1.00 15.24 6 1606 O SER A 200 19.994 77.917 16.741 1.00 11.79 8  
1565 CE1 PHE A 194 39.688 72.942 17.460 1.00 11.26 6 1607 CB SER A 200 21.636 80.012 15.731 1.00 14.77 6  
1566 CE2 PHE A 194 41.871 72.533 16.574 1.00 12.49 6 1608 OG SER A 200 20.723 81.011 16.249 1.00 13.69 8  
1567 CZ PHE A 194 40.860 72.181 17.450 1.00 12.03 6 1609 N GLN A 201 20.786 78.294 18.837 1.00 10.61 7  
1568 N SER A 195 38.283 77.497 15.895 1.00 10.73 7 1610 CA GLN A 201 19.599 77.668 19.473 1.00 11.55 6  
1569 CA SER A 195 37.097 77.782 16.704 1.00 11.52 6 1611 C GLN A 201 18.421 78.648 19.371 1.00 11.79 6  
1570 C SER A 195 36.081 76.649 16.423 1.00 11.92 6 1612 O GLN A 201 17.305 78.161 19.700 1.00 12.43 8  
1571 O SER A 195 36.284 75.902 15.519 1.00 10.36 8 1613 CB GLN A 201 19.852 77.359 20.969 1.00 11.94 6  
1572 CB SER A 195 36.416 79.059 16.186 1.00 16.30 6 1614 CG GLN A 201 21.042 76.370 21.151 1.00 10.05 6  
1573 OG SER A 195 37.442 80.119 16.216 1.00 22.79 8 1615 CD GLN A 201 22.393 77.086 21.126 1.00 10.84 6  
1574 N LEU A 196 35.060 76.594 17.262 1.00 12.22 7 1616 OE1 GLN A 201 22.499 78.298 21.208 1.00 11.60 8  
1575 CA LEU A 196 34.007 75.622 17.060 1.00 12.16 6 1617 NE2 GLN A 201 23.465 76.231 21.079 1.00 9.83 7  
1576 C LEU A 196 32.756 76.384 16.584 1.00 7.60 6 1618 N GLU A 202 18.590 79.860 18.862 1.00 10.41 7  
1577 O LEU A 196 32.364 77.416 17.112 1.00 13.16 8 1619 CA GLU A 202 17.434 80.763 18.667 1.00 11.55 6  
1578 CB LEU A 196 33.660 74.883 18.410 1.00 10.95 6 1620 C GLU A 202 16.849 80.531 17.277 1.00 14.51 6  
1579 CG LEU A 196 34.880 74.298 19.107 1.00 10.75 6 1621 O GLU A 202 15.856 81.166 16.903 1.00 16.57 8  
1580 CD1 LEU A 196 34.439 73.454 20.334 1.00 11.59 6 1622 CB GLU A 202 17.877 82.226 18.875 1.00 10.69 6  
1581 CD2 LEU A 196 35.719 73.384 18.134 1.00 12.48 6 1623 CG GLU A 202 18.522 82.442 20.252 1.00 9.01 6  
1582 N ALA A 197 32.139 75.877 15.481 1.00 9.97 7 1624 CD GLU A 202 20.002 82.069 20.330 1.00 12.78 6  
1583 CA ALA A 197 30.995 76.637 14.905 1.00 10.64 6 1625 OE1 GLU A 202 20.680 82.031 19.299 1.00 16.62 8  
1584 C ALA A 197 29.788 76.658 15.830 1.00 14.16 6 1626 OE2 GLU A 202 20.457 81.782 21.434 1.00 12.31 8  
1585 O ALA A 197 29.362 75.622 16.314 1.00 11.22 8 1627 N ASN A 203 17.507 79.704 16.435 1.00 11.04 7  
1586 CB ALA A 197 30.629 75.928 13.565 1.00 10.95 6 1628 CA ASN A 203 16.939 79.318 15.142 1.00 10.64 6  
1587 N ASP A 198 29.429 77.869 16.236 1.00 10.28 7 1629 C ASN A 203 16.020 78.098 15.372 1.00 13.48 6  
1588 CA ASP A 198 28.459 78.009 17.350 1.00 10.50 6 1630 O ASN A 203 16.441 77.148 16.008 1.00 12.81 8  
1589 C ASP A 198 27.030 77.880 16.795 1.00 11.99 6 1631 CB ASN A 203 18.105 78.892 14.217 1.00 11.71 6  
1590 O ASP A 198 26.607 78.731 15.993 1.00 13.33 8 1632 CG ASN A 203 17.604 78.307 12.930 1.00 15.36 6  
1591 CB ASP A 198 28.744 79.433 17.900 1.00 12.29 6 1633 OD1 ASN A 203 17.271 77.124 12.838 1.00 15.37 8  
1592 CG ASP A 198 28.236 79.529 19.353 1.00 10.72 6 1634 ND2 ASN A 203 17.611 79.108 11.829 1.00 15.33 7  
1593 OD1 ASP A 198 28.683 78.683 20.172 1.00 11.33 8 1635 N GLY A 204 14.797 78.219 14.831 1.00 13.94 7  
1594 OD2 ASP A 198 27.401 80.452 19.671 1.00 10.45 8 1636 CA GLY A 204 13.813 77.115 15.175 1.00 14.96 6  
1595 N LEU A 199 26.310 76.847 17.247 1.00 10.29 7 1637 C GLY A 204 14.202 75.766 14.593 1.00 12.98 6  
1596 CA LEU A 199 24.927 76.690 16.763 1.00 8.80 6 1638 O GLY A 204 13.891 74.775 15.243 1.00 14.33 8  
1597 C LEU A 199 24.086 77.821 17.321 1.00 9.88 6 1639 N THR A 205 14.802 75.705 13.401 1.00 11.88 7  
1598 O LEU A 199 24.246 78.320 18.449 1.00 11.27 8 1640 CA THR A 205 15.279 74.405 12.894 1.00 12.45 6  
1599 CB LEU A 199 24.452 75.296 17.279 1.00 9.52 6 1641 C THR A 205 16.275 73.780 13.856 1.00 11.35 6



|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1726 | CD  | GLN A 216 | 17.856 | 59.162 | 17.261 | 1.00 | 18.32 | 6 | 1768 | N   | ASP A 223 | 19.009 | 57.376 | 30.709 | 1.00 | 11.67 | 7 |
| 1727 | OE1 | GLN A 216 | 18.762 | 59.976 | 16.980 | 1.00 | 21.98 | 8 | 1769 | CA  | ASP A 223 | 18.391 | 57.768 | 31.951 | 1.00 | 10.83 | 6 |
| 1728 | NE2 | GLN A 216 | 17.392 | 58.348 | 16.335 | 1.00 | 19.07 | 7 | 1770 | C   | ASP A 223 | 18.621 | 59.249 | 32.306 | 1.00 | 12.58 | 6 |
| 1729 | N   | GLN A 217 | 17.996 | 60.043 | 22.269 | 1.00 | 11.16 | 7 | 1771 | O   | ASP A 223 | 18.116 | 59.667 | 33.356 | 1.00 | 11.47 | 8 |
| 1730 | CA  | LEU A 217 | 18.781 | 59.317 | 23.261 | 1.00 | 11.02 | 6 | 1772 | CB  | ASP A 223 | 18.997 | 56.964 | 33.123 | 1.00 | 9.67  | 6 |
| 1731 | C   | LEU A 217 | 17.885 | 58.756 | 24.396 | 1.00 | 10.47 | 6 | 1773 | CG  | ASP A 223 | 18.744 | 55.469 | 32.925 | 1.00 | 12.72 | 6 |
| 1732 | O   | LEU A 217 | 18.106 | 57.631 | 24.754 | 1.00 | 13.19 | 8 | 1774 | OD1 | ASP A 223 | 17.554 | 55.095 | 33.224 | 1.00 | 15.35 | 8 |
| 1733 | CB  | LEU A 217 | 19.847 | 60.252 | 23.876 | 1.00 | 12.00 | 6 | 1775 | OD2 | ASP A 223 | 19.610 | 54.686 | 32.482 | 1.00 | 10.77 | 8 |
| 1734 | CG  | LEU A 217 | 20.974 | 60.577 | 22.859 | 1.00 | 10.07 | 6 | 1776 | N   | GLY A 224 | 19.186 | 59.972 | 31.348 | 1.00 | 11.00 | 7 |
| 1735 | CD1 | LEU A 217 | 21.770 | 61.789 | 23.418 | 1.00 | 10.56 | 6 | 1777 | CA  | GLY A 224 | 19.393 | 61.413 | 31.651 | 1.00 | 11.62 | 6 |
| 1736 | CD2 | LEU A 217 | 21.953 | 59.383 | 22.787 | 1.00 | 12.18 | 6 | 1778 | C   | GLY A 224 | 20.641 | 61.861 | 30.809 | 1.00 | 9.62  | 6 |
| 1737 | N   | VAL A 218 | 16.940 | 59.584 | 24.844 | 1.00 | 10.50 | 7 | 1779 | O   | GLY A 224 | 21.069 | 61.107 | 29.928 | 1.00 | 9.69  | 8 |
| 1738 | CA  | VAL A 218 | 16.027 | 59.030 | 25.884 | 1.00 | 14.12 | 6 | 1780 | N   | LEU A 225 | 20.869 | 63.123 | 30.983 | 1.00 | 10.32 | 7 |
| 1739 | C   | VAL A 218 | 15.114 | 57.918 | 25.304 | 1.00 | 12.90 | 6 | 1781 | CA  | LEU A 225 | 21.962 | 63.749 | 30.177 | 1.00 | 9.63  | 6 |
| 1740 | O   | VAL A 218 | 14.914 | 56.898 | 25.978 | 1.00 | 14.29 | 8 | 1782 | C   | LEU A 225 | 22.828 | 64.566 | 31.128 | 1.00 | 10.99 | 6 |
| 1741 | CB  | VAL A 218 | 15.121 | 60.168 | 26.376 | 1.00 | 11.91 | 6 | 1783 | O   | LEU A 225 | 22.356 | 65.110 | 32.097 | 1.00 | 10.86 | 8 |
| 1742 | CG1 | VAL A 218 | 14.131 | 59.671 | 27.428 | 1.00 | 14.89 | 6 | 1784 | CB  | LEU A 225 | 21.389 | 64.780 | 29.172 | 1.00 | 9.89  | 6 |
| 1743 | CG2 | VAL A 218 | 16.045 | 61.169 | 27.107 | 1.00 | 14.59 | 6 | 1785 | CG  | LEU A 225 | 20.424 | 64.212 | 28.122 | 1.00 | 10.00 | 6 |
| 1744 | N   | ALA A 219 | 14.717 | 57.992 | 24.051 | 1.00 | 14.93 | 7 | 1786 | CD1 | LEU A 225 | 19.806 | 65.361 | 27.279 | 1.00 | 12.69 | 6 |
| 1745 | CA  | ALA A 219 | 13.868 | 56.915 | 23.478 | 1.00 | 14.21 | 6 | 1787 | CD2 | LEU A 225 | 21.003 | 63.092 | 27.243 | 1.00 | 13.97 | 6 |
| 1746 | C   | ALA A 219 | 14.647 | 55.619 | 23.377 | 1.00 | 16.64 | 6 | 1788 | N   | ARG A 226 | 24.135 | 64.671 | 30.790 | 1.00 | 10.52 | 7 |
| 1747 | O   | ALA A 219 | 14.072 | 54.517 | 23.401 | 1.00 | 14.94 | 8 | 1789 | CA  | ARG A 226 | 24.993 | 65.777 | 31.295 | 1.00 | 9.01  | 6 |
| 1748 | CB  | ALA A 219 | 13.379 | 57.270 | 22.059 | 1.00 | 15.54 | 6 | 1790 | C   | ARG A 226 | 25.093 | 66.744 | 30.110 | 1.00 | 10.97 | 6 |
| 1749 | N   | HIS A 220 | 15.959 | 55.702 | 23.258 | 1.00 | 12.54 | 7 | 1791 | O   | ARG A 226 | 25.628 | 66.348 | 29.083 | 1.00 | 10.94 | 8 |
| 1750 | CA  | HIS A 220 | 16.853 | 54.570 | 23.215 | 1.00 | 14.41 | 6 | 1792 | CB  | ARG A 226 | 26.337 | 65.159 | 31.691 | 1.00 | 9.10  | 6 |
| 1751 | C   | HIS A 220 | 17.305 | 54.124 | 24.611 | 1.00 | 12.25 | 6 | 1793 | CG  | ARG A 226 | 27.381 | 66.213 | 32.158 | 1.00 | 8.52  | 6 |
| 1752 | O   | HIS A 220 | 18.194 | 53.243 | 24.711 | 1.00 | 13.99 | 8 | 1794 | CD  | ARG A 226 | 28.248 | 66.648 | 30.956 | 1.00 | 9.82  | 6 |
| 1753 | CB  | HIS A 220 | 18.055 | 54.802 | 22.293 | 1.00 | 11.69 | 6 | 1795 | NE  | ARG A 226 | 29.438 | 67.400 | 31.425 | 1.00 | 9.22  | 7 |
| 1754 | CG  | HIS A 220 | 17.630 | 54.760 | 20.840 | 1.00 | 14.69 | 6 | 1796 | CZ  | ARG A 226 | 30.251 | 68.074 | 30.592 | 1.00 | 9.27  | 6 |
| 1755 | ND1 | HIS A 220 | 17.984 | 53.694 | 20.064 | 1.00 | 14.71 | 7 | 1797 | NH1 | ARG A 226 | 29.978 | 68.191 | 29.289 | 1.00 | 9.46  | 7 |
| 1756 | CD2 | HIS A 220 | 16.928 | 55.624 | 20.077 | 1.00 | 16.42 | 6 | 1798 | NH2 | ARG A 226 | 31.311 | 68.687 | 31.114 | 1.00 | 10.94 | 7 |
| 1757 | CE1 | HIS A 220 | 17.518 | 53.916 | 18.823 | 1.00 | 16.42 | 6 | 1799 | N   | ILE A 227 | 24.590 | 67.940 | 30.262 | 1.00 | 10.46 | 7 |
| 1758 | NE2 | HIS A 220 | 16.855 | 55.077 | 18.794 | 1.00 | 17.85 | 7 | 1800 | CA  | ILE A 227 | 24.553 | 68.901 | 29.124 | 1.00 | 7.87  | 6 |
| 1759 | N   | GLY A 221 | 16.735 | 54.666 | 25.655 | 1.00 | 11.47 | 7 | 1801 | C   | ILE A 227 | 25.807 | 69.751 | 29.238 | 1.00 | 8.86  | 6 |
| 1760 | CA  | GLY A 221 | 16.964 | 54.129 | 26.999 | 1.00 | 11.21 | 6 | 1802 | O   | ILE A 227 | 26.042 | 70.450 | 30.199 | 1.00 | 11.29 | 8 |
| 1761 | C   | GLY A 221 | 17.655 | 55.060 | 27.965 | 1.00 | 13.22 | 6 | 1803 | CB  | ILE A 227 | 23.295 | 69.783 | 29.269 | 1.00 | 9.62  | 6 |
| 1762 | O   | GLY A 221 | 17.875 | 54.635 | 29.095 | 1.00 | 13.24 | 8 | 1804 | CG1 | ILE A 227 | 22.096 | 68.814 | 29.378 | 1.00 | 10.28 | 6 |
| 1763 | N   | ALA A 222 | 18.297 | 56.111 | 27.426 | 1.00 | 12.29 | 7 | 1805 | CG2 | ILE A 227 | 23.196 | 70.601 | 27.964 | 1.00 | 11.21 | 6 |
| 1764 | CA  | ALA A 222 | 19.139 | 56.912 | 28.356 | 1.00 | 14.03 | 6 | 1806 | CD1 | ILE A 227 | 20.743 | 69.547 | 29.412 | 1.00 | 15.31 | 6 |
| 1765 | C   | ALA A 222 | 18.325 | 57.381 | 29.553 | 1.00 | 13.32 | 6 | 1807 | N   | ASP A 228 | 26.544 | 69.672 | 28.125 | 1.00 | 9.30  | 7 |
| 1766 | O   | ALA A 222 | 17.138 | 57.794 | 29.459 | 1.00 | 10.61 | 8 | 1808 | CA  | ASP A 228 | 27.846 | 70.399 | 28.079 | 1.00 | 9.30  | 6 |
| 1767 | CB  | ALA A 222 | 19.700 | 58.136 | 27.618 | 1.00 | 12.95 | 6 | 1809 | C   | ASP A 228 | 27.672 | 71.915 | 27.904 | 1.00 | 9.50  | 6 |

|      |     |           |        |        |        |      |       |   |      |               |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 1810 | O   | ASP A 228 | 26.757 | 72.338 | 27.189 | 1.00 | 9.88  | 8 | 1852 | CD1 PHE A 233 | 24.335 | 75.588 | 25.559 | 1.00 | 12.13 | 6 |
| 1811 | CB  | ASP A 228 | 28.521 | 69.865 | 26.769 | 1.00 | 9.23  | 6 | 1853 | CD2 PHE A 233 | 22.023 | 76.331 | 25.466 | 1.00 | 11.40 | 6 |
| 1812 | CG  | ASP A 228 | 29.904 | 70.442 | 26.587 | 1.00 | 10.24 | 6 | 1854 | CE1 PHE A 233 | 23.982 | 74.503 | 26.347 | 1.00 | 12.18 | 6 |
| 1813 | OD1 | ASP A 228 | 30.725 | 70.228 | 27.505 | 1.00 | 10.28 | 8 | 1855 | CE2 PHE A 233 | 21.642 | 75.219 | 26.237 | 1.00 | 10.50 | 6 |
| 1814 | OD2 | ASP A 228 | 30.208 | 71.128 | 25.574 | 1.00 | 9.89  | 8 | 1856 | CZ PHE A 233  | 22.629 | 74.340 | 26.657 | 1.00 | 11.82 | 6 |
| 1815 | N   | ALA A 229 | 28.575 | 72.633 | 28.582 | 1.00 | 8.93  | 7 | 1857 | N ASN A 234   | 22.051 | 80.148 | 25.349 | 1.00 | 12.13 | 7 |
| 1816 | CA  | ALA A 229 | 28.745 | 74.068 | 28.257 | 1.00 | 9.72  | 6 | 1858 | CA ASN A 234  | 21.093 | 80.799 | 26.253 | 1.00 | 8.31  | 6 |
| 1817 | C   | ALA A 229 | 27.455 | 74.868 | 28.324 | 1.00 | 10.58 | 6 | 1859 | C ASN A 234   | 20.367 | 79.859 | 27.214 | 1.00 | 9.45  | 6 |
| 1818 | O   | ALA A 229 | 27.123 | 75.695 | 27.464 | 1.00 | 10.73 | 8 | 1860 | O ASN A 234   | 20.112 | 78.722 | 26.829 | 1.00 | 9.94  | 8 |
| 1819 | CB  | ALA A 229 | 29.355 | 74.180 | 26.841 | 1.00 | 9.90  | 6 | 1861 | CB ASN A 234  | 20.132 | 81.662 | 25.369 | 1.00 | 10.71 | 6 |
| 1820 | N   | VAL A 230 | 26.729 | 74.708 | 29.487 | 1.00 | 9.05  | 7 | 1862 | CG ASN A 234  | 18.981 | 80.871 | 24.740 | 1.00 | 12.93 | 6 |
| 1821 | CA  | VAL A 230 | 25.421 | 75.392 | 29.548 | 1.00 | 9.09  | 6 | 1863 | OD1 ASN A 234 | 18.070 | 80.516 | 25.519 | 1.00 | 12.50 | 8 |
| 1822 | C   | VAL A 230 | 25.547 | 76.905 | 29.753 | 1.00 | 10.83 | 6 | 1864 | ND2 ASN A 234 | 18.975 | 80.590 | 23.448 | 1.00 | 10.79 | 7 |
| 1823 | O   | VAL A 230 | 24.587 | 77.636 | 29.573 | 1.00 | 12.48 | 8 | 1865 | N SER A 235   | 20.023 | 80.451 | 28.374 | 1.00 | 10.78 | 7 |
| 1824 | CB  | VAL A 230 | 24.469 | 74.836 | 30.634 | 1.00 | 10.80 | 6 | 1866 | CA SER A 235  | 19.401 | 79.586 | 29.396 | 1.00 | 8.67  | 6 |
| 1825 | CG1 | VAL A 230 | 24.119 | 73.389 | 30.262 | 1.00 | 9.84  | 6 | 1867 | C SER A 235   | 17.906 | 79.375 | 29.177 | 1.00 | 11.06 | 6 |
| 1826 | CG2 | VAL A 230 | 25.084 | 74.934 | 32.047 | 1.00 | 11.19 | 6 | 1868 | O SER A 235   | 17.399 | 78.402 | 29.759 | 1.00 | 11.56 | 8 |
| 1827 | N   | LYS A 231 | 26.753 | 77.312 | 30.189 | 1.00 | 9.10  | 7 | 1869 | CB ASER A 235 | 19.594 | 80.196 | 30.792 | 0.60 | 11.41 | 6 |
| 1828 | CA  | LYS A 231 | 26.988 | 78.763 | 30.234 | 1.00 | 7.91  | 6 | 1870 | OG ASER A 235 | 20.974 | 80.269 | 31.098 | 0.60 | 10.81 | 8 |
| 1829 | C   | LYS A 231 | 27.304 | 79.391 | 28.883 | 1.00 | 11.01 | 6 | 1869 | CB BSER A 235 | 19.679 | 80.067 | 30.817 | 0.40 | 10.03 | 6 |
| 1830 | O   | LYS A 231 | 27.398 | 80.604 | 28.809 | 1.00 | 13.02 | 8 | 1870 | OG BSER A 235 | 19.311 | 81.423 | 30.914 | 0.40 | 7.85  | 8 |
| 1831 | CB  | LYS A 231 | 28.173 | 79.043 | 31.209 | 1.00 | 10.48 | 6 | 1871 | N GLY A 236   | 17.301 | 80.140 | 28.312 | 1.00 | 10.81 | 7 |
| 1832 | CG  | LYS A 231 | 29.567 | 78.801 | 30.602 | 1.00 | 10.63 | 6 | 1872 | CA GLY A 236  | 15.906 | 79.857 | 27.882 | 1.00 | 11.83 | 6 |
| 1833 | CD  | LYS A 231 | 30.599 | 78.817 | 31.758 | 1.00 | 13.70 | 6 | 1873 | C GLY A 236   | 15.821 | 78.448 | 27.289 | 1.00 | 12.34 | 6 |
| 1834 | CE  | LYS A 231 | 30.937 | 80.205 | 32.236 | 1.00 | 13.75 | 6 | 1874 | O GLY A 236   | 14.942 | 77.638 | 27.552 | 1.00 | 11.07 | 8 |
| 1835 | NZ  | LYS A 231 | 32.215 | 80.157 | 33.104 | 1.00 | 11.49 | 7 | 1875 | N PHE A 237   | 16.742 | 78.158 | 26.370 | 1.00 | 10.75 | 7 |
| 1836 | N   | HIS A 232 | 27.364 | 78.589 | 27.814 | 1.00 | 9.37  | 7 | 1876 | CA PHE A 237  | 16.793 | 76.864 | 25.702 | 1.00 | 9.60  | 6 |
| 1837 | CA  | HIS A 232 | 27.744 | 79.081 | 26.480 | 1.00 | 12.72 | 6 | 1877 | C PHE A 237   | 17.034 | 75.738 | 26.715 | 1.00 | 10.90 | 6 |
| 1838 | C   | HIS A 232 | 26.576 | 79.044 | 25.537 | 1.00 | 12.48 | 6 | 1878 | O PHE A 237   | 16.476 | 74.641 | 26.526 | 1.00 | 10.74 | 8 |
| 1839 | O   | HIS A 232 | 26.698 | 79.505 | 24.388 | 1.00 | 9.62  | 8 | 1879 | CB PHE A 237  | 17.714 | 76.891 | 24.467 | 1.00 | 12.14 | 6 |
| 1840 | CB  | HIS A 232 | 28.849 | 78.129 | 25.915 | 1.00 | 9.94  | 6 | 1880 | CG PHE A 237  | 17.642 | 75.595 | 23.691 | 1.00 | 12.02 | 6 |
| 1841 | CG  | HIS A 232 | 30.145 | 78.345 | 26.709 | 1.00 | 9.35  | 6 | 1881 | CD1 PHE A 237 | 16.442 | 75.242 | 23.048 | 1.00 | 12.55 | 6 |
| 1842 | ND1 | HIS A 232 | 30.780 | 79.598 | 26.674 | 1.00 | 11.03 | 7 | 1882 | CD2 PHE A 237 | 18.751 | 74.740 | 23.659 | 1.00 | 11.64 | 6 |
| 1843 | CD2 | HIS A 232 | 30.803 | 77.530 | 27.554 | 1.00 | 11.85 | 6 | 1883 | CE1 PHE A 237 | 16.367 | 74.046 | 22.358 | 1.00 | 12.60 | 6 |
| 1844 | CE1 | HIS A 232 | 31.838 | 79.483 | 27.513 | 1.00 | 12.22 | 6 | 1884 | CE2 PHE A 237 | 18.634 | 73.533 | 22.952 | 1.00 | 11.39 | 6 |
| 1845 | NE2 | HIS A 232 | 31.882 | 78.243 | 28.049 | 1.00 | 11.68 | 7 | 1885 | CZ PHE A 237  | 17.468 | 73.200 | 22.301 | 1.00 | 13.43 | 6 |
| 1846 | N   | PHE A 233 | 25.342 | 78.757 | 25.941 | 1.00 | 9.67  | 7 | 1886 | N SER A 238   | 17.965 | 75.939 | 27.658 | 1.00 | 10.56 | 7 |
| 1847 | CA  | PHE A 233 | 24.165 | 78.957 | 25.062 | 1.00 | 10.57 | 6 | 1887 | CA SER A 238  | 18.119 | 74.844 | 28.637 | 1.00 | 11.43 | 6 |
| 1848 | C   | PHE A 233 | 23.015 | 79.437 | 25.991 | 1.00 | 9.21  | 6 | 1888 | C SER A 238   | 16.762 | 74.489 | 29.289 | 1.00 | 10.24 | 6 |
| 1849 | O   | PHE A 233 | 23.073 | 79.254 | 27.225 | 1.00 | 11.50 | 8 | 1889 | O SER A 238   | 16.416 | 73.312 | 29.442 | 1.00 | 10.58 | 8 |
| 1850 | CB  | PHE A 233 | 23.792 | 77.705 | 24.296 | 1.00 | 9.50  | 6 | 1890 | CB SER A 238  | 19.069 | 75.303 | 29.776 | 1.00 | 11.86 | 6 |
| 1851 | CG  | PHE A 233 | 23.382 | 76.523 | 25.145 | 1.00 | 10.66 | 6 | 1891 | OG SER A 238  | 20.432 | 75.070 | 29.404 | 1.00 | 12.16 | 8 |

|      |     |           |        |        |        |      |       |   |      |     |            |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|------------|--------|--------|--------|------|-------|---|
| 1892 | N   | LYS A 239 | 16.053 | 75.523 | 29.757 | 1.00 | 10.06 | 7 | 1934 | CD  | LYS A 244  | 9.398  | 70.400 | 24.483 | 1.00 | 13.14 | 6 |
| 1893 | CA  | LYS A 239 | 14.749 | 75.262 | 30.433 | 1.00 | 10.43 | 6 | 1935 | CE  | LYS A 244  | 9.129  | 71.869 | 24.133 | 1.00 | 13.82 | 6 |
| 1894 | C   | LYS A 239 | 13.712 | 74.684 | 29.505 | 1.00 | 10.95 | 6 | 1936 | NZ  | LYS A 244  | 9.582  | 72.780 | 25.269 | 1.00 | 12.11 | 7 |
| 1895 | O   | LYS A 239 | 13.006 | 73.718 | 29.879 | 1.00 | 11.91 | 8 | 1937 | N   | LEU A 245  | 12.213 | 67.068 | 27.593 | 1.00 | 11.20 | 7 |
| 1896 | CB  | LYS A 239 | 14.259 | 76.598 | 31.123 | 1.00 | 8.56  | 6 | 1938 | CA  | LEU A 245  | 12.730 | 65.762 | 28.039 | 1.00 | 11.98 | 6 |
| 1897 | CG  | LYS A 239 | 12.889 | 76.329 | 31.861 | 1.00 | 12.08 | 6 | 1939 | C   | LEU A 245  | 11.936 | 65.200 | 29.205 | 1.00 | 12.96 | 6 |
| 1898 | CD  | LYS A 239 | 12.577 | 77.644 | 32.648 | 1.00 | 11.14 | 6 | 1940 | O   | LEU A 245  | 11.665 | 63.996 | 29.219 | 1.00 | 12.16 | 8 |
| 1899 | CE  | LYS A 239 | 11.131 | 77.442 | 33.240 | 1.00 | 11.14 | 6 | 1941 | CB  | LEU A 245  | 14.221 | 65.961 | 28.461 | 1.00 | 10.88 | 6 |
| 1900 | NZ  | LYS A 239 | 10.797 | 78.668 | 34.098 | 1.00 | 10.40 | 7 | 1942 | CG  | LEU A 245  | 15.091 | 66.282 | 27.206 | 1.00 | 15.60 | 6 |
| 1901 | N   | SER A 240 | 13.600 | 75.153 | 28.279 | 1.00 | 9.61  | 7 | 1943 | CD1 | LEU A 245  | 16.493 | 66.701 | 27.692 | 1.00 | 14.87 | 6 |
| 1902 | CA  | SER A 240 | 12.611 | 74.583 | 27.330 | 1.00 | 9.08  | 6 | 1944 | CD2 | LEU A 245  | 15.227 | 65.052 | 26.282 | 1.00 | 19.24 | 6 |
| 1903 | C   | SER A 240 | 13.006 | 73.207 | 26.957 | 1.00 | 10.90 | 6 | 1945 | N   | TYR A 246  | 11.480 | 66.037 | 30.136 | 1.00 | 11.31 | 7 |
| 1904 | O   | SER A 240 | 12.160 | 72.320 | 26.790 | 1.00 | 10.77 | 8 | 1946 | CA  | TYR A 246  | 10.676 | 65.529 | 31.258 | 1.00 | 11.13 | 6 |
| 1905 | CB  | SER A 240 | 12.560 | 75.572 | 26.136 | 1.00 | 11.38 | 6 | 1947 | C   | TYR A 246  | 9.294  | 65.090 | 30.770 | 1.00 | 11.59 | 6 |
| 1906 | OG  | SER A 240 | 11.488 | 75.039 | 25.266 | 1.00 | 12.68 | 8 | 1948 | O   | TYR A 246  | 8.674  | 64.306 | 31.500 | 1.00 | 13.03 | 8 |
| 1907 | N   | LEU A 241 | 14.300 | 72.896 | 26.747 | 1.00 | 10.43 | 7 | 1949 | CB  | TYR A 246  | 10.582 | 66.586 | 32.359 | 1.00 | 12.53 | 6 |
| 1908 | CA  | LEU A 241 | 14.726 | 71.560 | 26.389 | 1.00 | 10.29 | 6 | 1950 | CG  | TYR A 246  | 11.928 | 66.907 | 32.995 | 1.00 | 9.85  | 6 |
| 1909 | C   | LEU A 241 | 14.420 | 70.599 | 27.539 | 1.00 | 11.73 | 6 | 1951 | CD1 | TYR A 246  | 12.882 | 65.941 | 33.210 | 1.00 | 11.79 | 6 |
| 1910 | O   | LEU A 241 | 13.924 | 69.507 | 27.303 | 1.00 | 11.15 | 8 | 1952 | CD2 | TYR A 246  | 12.163 | 68.228 | 33.408 | 1.00 | 10.52 | 6 |
| 1911 | CB  | LEU A 241 | 16.255 | 71.582 | 26.077 | 1.00 | 10.07 | 6 | 1953 | CE1 | TYR A 246  | 14.103 | 66.245 | 33.830 | 1.00 | 11.71 | 6 |
| 1912 | CG  | LEU A 241 | 16.816 | 70.170 | 25.829 | 1.00 | 12.71 | 6 | 1954 | CE2 | TYR A 246  | 13.379 | 68.569 | 34.021 | 1.00 | 10.59 | 6 |
| 1913 | CD1 | LEU A 241 | 16.205 | 69.502 | 24.577 | 1.00 | 13.39 | 6 | 1955 | CZ  | TYR A 246  | 14.319 | 67.562 | 34.208 | 1.00 | 11.60 | 6 |
| 1914 | CD2 | LEU A 241 | 18.333 | 70.350 | 25.611 | 1.00 | 12.90 | 6 | 1956 | OH  | TYR A 246  | 15.536 | 67.856 | 34.816 | 1.00 | 11.49 | 8 |
| 1915 | N   | ALA A 242 | 14.710 | 71.055 | 28.778 | 1.00 | 11.25 | 7 | 1957 | N   | GLN A 247  | 8.769  | 65.623 | 29.672 | 1.00 | 12.54 | 7 |
| 1916 | CA  | ALA A 242 | 14.427 | 70.181 | 29.912 | 1.00 | 10.06 | 6 | 1958 | CA  | GLN A 247  | 7.501  | 65.088 | 29.112 | 1.00 | 13.07 | 6 |
| 1917 | C   | ALA A 242 | 12.923 | 69.852 | 29.969 | 1.00 | 10.68 | 6 | 1959 | C   | GLN A 247  | 7.677  | 63.690 | 28.587 | 1.00 | 13.75 | 6 |
| 1918 | O   | ALA A 242 | 12.565 | 68.703 | 30.215 | 1.00 | 10.97 | 8 | 1960 | O   | GLN A 247  | 6.712  | 62.875 | 28.651 | 1.00 | 16.16 | 8 |
| 1919 | CB  | ALA A 242 | 14.910 | 70.889 | 31.196 | 1.00 | 10.49 | 6 | 1961 | CB  | GLN A 247  | 7.016  | 66.001 | 27.940 | 1.00 | 12.33 | 6 |
| 1920 | N   | ASP A 243 | 12.062 | 70.870 | 29.712 | 1.00 | 10.40 | 7 | 1962 | CG  | GLN A 247  | 6.530  | 67.357 | 28.518 | 1.00 | 13.62 | 6 |
| 1921 | CA  | ASP A 243 | 10.609 | 70.595 | 29.694 | 1.00 | 11.54 | 6 | 1963 | CD  | GLN A 247  | 6.016  | 68.220 | 27.397 | 1.00 | 16.89 | 6 |
| 1922 | C   | ASP A 243 | 10.365 | 69.448 | 28.700 | 1.00 | 12.78 | 6 | 1964 | OE1 | GLN A 247  | 5.355  | 67.699 | 26.462 | 1.00 | 18.89 | 8 |
| 1923 | O   | ASP A 243 | 9.636  | 68.474 | 29.006 | 1.00 | 12.31 | 8 | 1965 | NE2 | GLN A 247  | 6.372  | 69.518 | 27.387 | 1.00 | 14.76 | 7 |
| 1924 | CB  | ASP A 243 | 9.930  | 71.904 | 29.186 | 1.00 | 11.95 | 6 | 1966 | N   | LYS A 248  | 8.881  | 63.349 | 28.162 | 1.00 | 14.17 | 7 |
| 1925 | CG  | ASP A 243 | 8.507  | 71.717 | 28.674 | 1.00 | 13.21 | 6 | 1967 | CA  | LYS A 248  | 9.163  | 61.979 | 27.702 | 1.00 | 15.18 | 6 |
| 1926 | OD1 | ASP A 243 | 7.668  | 71.113 | 29.422 | 1.00 | 12.98 | 8 | 1968 | C   | LYS A 248  | 9.328  | 61.000 | 28.836 | 1.00 | 15.52 | 6 |
| 1927 | OD2 | ASP A 243 | 8.223  | 72.178 | 27.546 | 1.00 | 12.92 | 8 | 1969 | O   | LYS A 248  | 8.839  | 59.868 | 28.746 | 1.00 | 16.45 | 8 |
| 1928 | N   | LYS A 244 | 10.825 | 69.536 | 27.451 | 1.00 | 10.42 | 7 | 1970 | CB  | ALYS A 248 | 10.397 | 61.994 | 26.793 | 0.50 | 13.40 | 6 |
| 1929 | CA  | LYS A 244 | 10.523 | 68.449 | 26.484 | 1.00 | 10.94 | 6 | 1971 | CG  | ALYS A 248 | 10.116 | 62.793 | 25.528 | 0.50 | 14.14 | 6 |
| 1930 | C   | LYS A 244 | 10.997 | 67.097 | 26.998 | 1.00 | 13.31 | 6 | 1972 | CD  | ALYS A 248 | 8.958  | 62.165 | 24.749 | 0.50 | 17.69 | 6 |
| 1931 | O   | LYS A 244 | 10.349 | 66.061 | 26.763 | 1.00 | 12.24 | 8 | 1973 | CE  | ALYS A 248 | 8.449  | 63.068 | 23.657 | 0.50 | 18.41 | 6 |
| 1932 | CB  | LYS A 244 | 11.232 | 68.728 | 25.122 | 1.00 | 11.69 | 6 | 1974 | NZ  | ALYS A 248 | 7.682  | 62.378 | 22.577 | 0.50 | 25.68 | 7 |
| 1933 | CG  | LYS A 244 | 10.924 | 70.142 | 24.580 | 1.00 | 14.16 | 6 | 1970 | CB  | BLYS A 248 | 10.414 | 62.030 | 26.816 | 0.50 | 17.60 | 6 |



|      |     |      |   |     |        |        |        |      |       |   |      |     |     |   |     |        |        |        |      |       |   |
|------|-----|------|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 1971 | CG  | BLYS | A | 248 | 10.840 | 60.676 | 26.292 | 0.50 | 22.20 | 6 | 2013 | C   | LEU | A | 253 | 20.498 | 67.083 | 34.913 | 1.00 | 9.94  | 6 |
| 1972 | CD  | BLYS | A | 248 | 11.561 | 60.755 | 24.977 | 0.50 | 29.85 | 6 | 2014 | O   | LEU | A | 253 | 20.094 | 67.647 | 35.914 | 1.00 | 11.26 | 8 |
| 1973 | CE  | BLYS | A | 248 | 11.495 | 59.497 | 24.150 | 0.50 | 18.09 | 6 | 2015 | CB  | LEU | A | 253 | 18.694 | 67.378 | 33.282 | 1.00 | 8.72  | 6 |
| 1974 | NZ  | BLYS | A | 248 | 10.779 | 58.367 | 24.885 | 0.50 | 21.86 | 7 | 2016 | CG  | LEU | A | 253 | 17.749 | 66.766 | 32.216 | 1.00 | 10.91 | 6 |
| 1975 | N   | LYS  | A | 249 | 10.131 | 61.400 | 29.830 | 1.00 | 12.97 | 7 | 2017 | CD1 | LEU | A | 253 | 16.881 | 67.891 | 31.562 | 1.00 | 10.35 | 6 |
| 1976 | CA  | LYS  | A | 249 | 10.424 | 60.442 | 30.917 | 1.00 | 14.04 | 6 | 2018 | CD2 | LEU | A | 253 | 18.508 | 66.051 | 31.089 | 1.00 | 12.13 | 6 |
| 1977 | C   | LYS  | A | 249 | 10.983 | 61.213 | 32.084 | 1.00 | 11.94 | 6 | 2019 | N   | VAL | A | 254 | 21.761 | 67.179 | 34.422 | 1.00 | 11.23 | 7 |
| 1978 | O   | LYS  | A | 249 | 11.520 | 62.316 | 31.876 | 1.00 | 13.26 | 8 | 2020 | CA  | VAL | A | 254 | 22.750 | 68.015 | 35.077 | 1.00 | 11.09 | 6 |
| 1979 | CB  | LYS  | A | 249 | 11.514 | 59.423 | 30.462 | 1.00 | 15.09 | 6 | 2021 | C   | VAL | A | 254 | 23.423 | 68.807 | 33.921 | 1.00 | 10.26 | 6 |
| 1980 | CG  | LYS  | A | 249 | 11.674 | 58.358 | 31.542 | 1.00 | 15.17 | 6 | 2022 | O   | VAL | A | 254 | 23.707 | 68.196 | 32.892 | 1.00 | 10.32 | 8 |
| 1981 | CD  | LYS  | A | 249 | 12.552 | 57.175 | 31.147 | 1.00 | 23.08 | 6 | 2023 | CB  | VAL | A | 254 | 23.722 | 67.184 | 35.947 | 1.00 | 9.61  | 6 |
| 1982 | CE  | LYS  | A | 249 | 12.451 | 56.111 | 32.249 | 1.00 | 27.89 | 6 | 2024 | CG1 | VAL | A | 254 | 24.552 | 66.161 | 35.161 | 1.00 | 10.99 | 6 |
| 1983 | NZ  | LYS  | A | 249 | 13.149 | 54.836 | 31.875 | 1.00 | 36.10 | 7 | 2025 | CG2 | VAL | A | 254 | 24.688 | 68.131 | 36.685 | 1.00 | 11.22 | 6 |
| 1984 | N   | ASP  | A | 250 | 10.870 | 60.678 | 33.288 | 1.00 | 11.41 | 7 | 2026 | N   | GLY | A | 255 | 23.762 | 70.047 | 34.194 | 1.00 | 10.96 | 7 |
| 1985 | CA  | ASP  | A | 250 | 11.406 | 61.336 | 34.494 | 1.00 | 12.04 | 6 | 2027 | CA  | GLY | A | 255 | 24.492 | 70.879 | 33.243 | 1.00 | 11.43 | 6 |
| 1986 | C   | ASP  | A | 250 | 12.918 | 61.011 | 34.626 | 1.00 | 11.51 | 6 | 2028 | C   | GLY | A | 255 | 25.877 | 71.193 | 33.731 | 1.00 | 11.23 | 6 |
| 1987 | O   | ASP  | A | 250 | 13.348 | 60.354 | 35.546 | 1.00 | 13.89 | 8 | 2029 | O   | GLY | A | 255 | 26.095 | 71.404 | 34.967 | 1.00 | 10.31 | 8 |
| 1988 | CB  | ASP  | A | 250 | 10.638 | 60.891 | 35.728 | 1.00 | 11.54 | 6 | 2030 | N   | GLU | A | 256 | 26.828 | 71.308 | 32.765 | 1.00 | 10.72 | 7 |
| 1989 | CG  | ASP  | A | 250 | 10.618 | 59.405 | 36.030 | 1.00 | 15.08 | 6 | 2031 | CA  | GLU | A | 256 | 28.159 | 71.786 | 33.187 | 1.00 | 10.84 | 6 |
| 1990 | OD1 | ASP  | A | 250 | 10.695 | 58.618 | 35.085 | 1.00 | 15.58 | 8 | 2032 | C   | GLU | A | 256 | 28.236 | 73.315 | 33.013 | 1.00 | 11.33 | 6 |
| 1991 | OD2 | ASP  | A | 250 | 10.448 | 59.027 | 37.224 | 1.00 | 15.73 | 8 | 2033 | O   | GLU | A | 256 | 28.295 | 73.820 | 31.871 | 1.00 | 10.36 | 8 |
| 1992 | N   | ILE  | A | 251 | 13.644 | 61.541 | 33.607 | 1.00 | 11.19 | 7 | 2034 | CB  | GLU | A | 256 | 29.172 | 71.178 | 32.167 | 1.00 | 10.52 | 6 |
| 1993 | CA  | ILE  | A | 251 | 15.093 | 61.346 | 33.593 | 1.00 | 12.04 | 6 | 2035 | CG  | GLU | A | 256 | 30.603 | 71.617 | 32.605 | 1.00 | 10.70 | 6 |
| 1994 | C   | ILE  | A | 251 | 15.777 | 62.413 | 34.467 | 1.00 | 12.14 | 6 | 2036 | CD  | GLU | A | 256 | 31.442 | 72.059 | 31.414 | 1.00 | 11.32 | 6 |
| 1995 | O   | ILE  | A | 251 | 15.148 | 63.303 | 34.990 | 1.00 | 13.37 | 8 | 2037 | OE1 | GLU | A | 256 | 30.925 | 72.467 | 30.347 | 1.00 | 10.78 | 8 |
| 1996 | CB  | ILE  | A | 251 | 15.610 | 61.331 | 32.164 | 1.00 | 15.29 | 6 | 2038 | OE2 | GLU | A | 256 | 32.696 | 71.998 | 31.517 | 1.00 | 11.88 | 8 |
| 1997 | CG1 | ILE  | A | 251 | 14.988 | 62.477 | 31.361 | 1.00 | 23.77 | 6 | 2039 | N   | TRP | A | 257 | 28.173 | 74.038 | 34.120 | 1.00 | 9.79  | 7 |
| 1998 | CG2 | ILE  | A | 251 | 15.204 | 60.064 | 31.402 | 1.00 | 16.73 | 6 | 2040 | CA  | TRP | A | 257 | 28.409 | 75.480 | 34.158 | 1.00 | 9.57  | 6 |
| 1999 | CD1 | ILE  | A | 251 | 15.645 | 63.784 | 31.503 | 1.00 | 25.03 | 6 | 2041 | C   | TRP | A | 257 | 29.798 | 75.608 | 34.799 | 1.00 | 10.84 | 6 |
| 2000 | N   | PHE  | A | 252 | 17.122 | 62.248 | 34.639 | 1.00 | 9.99  | 7 | 2042 | O   | TRP | A | 257 | 29.908 | 75.560 | 36.037 | 1.00 | 10.82 | 8 |
| 2001 | CA  | PHE  | A | 252 | 17.885 | 63.182 | 35.420 | 1.00 | 9.59  | 6 | 2043 | CB  | TRP | A | 257 | 27.301 | 76.175 | 34.997 | 1.00 | 9.83  | 6 |
| 2002 | C   | PHE  | A | 252 | 18.690 | 64.105 | 34.501 | 1.00 | 11.26 | 6 | 2044 | CG  | TRP | A | 257 | 27.449 | 77.700 | 34.854 | 1.00 | 8.59  | 6 |
| 2003 | O   | PHE  | A | 252 | 19.347 | 63.587 | 33.596 | 1.00 | 12.38 | 8 | 2045 | CD1 | TRP | A | 257 | 28.566 | 78.442 | 35.196 | 1.00 | 12.90 | 6 |
| 2004 | CB  | PHE  | A | 252 | 18.916 | 62.372 | 36.275 | 1.00 | 13.00 | 6 | 2046 | CD2 | TRP | A | 257 | 26.431 | 78.592 | 34.412 | 1.00 | 10.35 | 6 |
| 2005 | CG  | PHE  | A | 252 | 19.748 | 63.290 | 37.145 | 1.00 | 11.27 | 6 | 2047 | NE1 | TRP | A | 257 | 28.295 | 79.753 | 34.937 | 1.00 | 12.55 | 7 |
| 2006 | CD1 | PHE  | A | 252 | 19.182 | 63.951 | 38.241 | 1.00 | 12.24 | 6 | 2048 | CE2 | TRP | A | 257 | 27.020 | 79.891 | 34.459 | 1.00 | 12.29 | 6 |
| 2007 | CD2 | PHE  | A | 252 | 21.094 | 63.494 | 36.838 | 1.00 | 12.52 | 6 | 2049 | CE3 | TRP | A | 257 | 25.124 | 78.425 | 33.946 | 1.00 | 13.94 | 6 |
| 2008 | CE1 | PHE  | A | 252 | 19.907 | 64.802 | 39.029 | 1.00 | 11.05 | 6 | 2050 | CZ2 | TRP | A | 257 | 26.317 | 81.041 | 34.055 | 1.00 | 10.73 | 6 |
| 2009 | CE2 | PHE  | A | 252 | 21.843 | 64.327 | 37.664 | 1.00 | 11.26 | 6 | 2051 | CZ3 | TRP | A | 257 | 24.385 | 79.544 | 33.527 | 1.00 | 13.32 | 6 |
| 2010 | CZ  | PHE  | A | 252 | 21.263 | 65.031 | 38.750 | 1.00 | 10.84 | 6 | 2052 | CH2 | TRP | A | 257 | 25.026 | 80.793 | 33.599 | 1.00 | 11.64 | 6 |
| 2011 | N   | LEU  | A | 253 | 18.740 | 65.389 | 34.772 | 1.00 | 12.09 | 7 | 2053 | N   | TYR | A | 258 | 30.831 | 75.725 | 33.986 | 1.00 | 11.79 | 7 |
| 2012 | CA  | LEU  | A | 253 | 19.592 | 66.278 | 33.936 | 1.00 | 9.30  | 6 | 2054 | CA  | TYR | A | 258 | 32.211 | 75.619 | 34.524 | 1.00 | 11.80 | 6 |

|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2055 | C   | TYR A 258 | 32.527 | 76.859 | 35.355 | 1.00 | 12.06 | 6 | 2097 | CA  | THR A 264 | 32.579 | 85.990 | 41.270 | 1.00 | 15.29 | 6 |
| 2056 | O   | TYR A 258 | 32.370 | 77.988 | 34.869 | 1.00 | 13.57 | 8 | 2098 | C   | THR A 264 | 31.378 | 86.647 | 40.599 | 1.00 | 14.14 | 6 |
| 2057 | CB  | TYR A 258 | 33.189 | 75.508 | 33.335 | 1.00 | 11.31 | 6 | 2099 | O   | THR A 264 | 30.225 | 86.490 | 41.019 | 1.00 | 15.14 | 8 |
| 2058 | CG  | TYR A 258 | 34.562 | 74.978 | 33.723 | 1.00 | 11.97 | 6 | 2100 | CB  | THR A 264 | 33.154 | 84.890 | 40.377 | 1.00 | 17.00 | 6 |
| 2059 | CD1 | TYR A 258 | 35.452 | 75.687 | 34.524 | 1.00 | 13.71 | 6 | 2101 | OG1 | THR A 264 | 32.185 | 83.864 | 40.214 | 1.00 | 17.20 | 8 |
| 2060 | CD2 | TYR A 258 | 34.932 | 73.734 | 33.234 | 1.00 | 11.78 | 6 | 2102 | CG2 | THR A 264 | 34.455 | 84.302 | 40.998 | 1.00 | 18.53 | 6 |
| 2061 | CE1 | TYR A 258 | 36.707 | 75.160 | 34.859 | 1.00 | 15.77 | 6 | 2103 | N   | ALA A 265 | 31.684 | 87.407 | 39.536 | 1.00 | 14.47 | 7 |
| 2062 | CE2 | TYR A 258 | 36.179 | 73.226 | 33.564 | 1.00 | 13.38 | 6 | 2104 | CA  | ALA A 265 | 30.579 | 88.206 | 38.957 | 1.00 | 16.68 | 6 |
| 2063 | CZ  | TYR A 258 | 37.037 | 73.908 | 34.376 | 1.00 | 16.44 | 6 | 2105 | C   | ALA A 265 | 29.455 | 87.387 | 38.348 | 1.00 | 14.50 | 6 |
| 2064 | OH  | TYR A 258 | 38.277 | 73.304 | 34.631 | 1.00 | 20.59 | 8 | 2106 | O   | ALA A 265 | 28.315 | 87.921 | 38.316 | 1.00 | 15.71 | 8 |
| 2065 | N   | GLY A 259 | 33.030 | 76.605 | 36.550 | 1.00 | 9.86  | 7 | 2107 | CB  | ALA A 265 | 31.153 | 89.034 | 37.793 | 1.00 | 18.93 | 6 |
| 2066 | CA  | GLY A 259 | 33.584 | 77.705 | 37.361 | 1.00 | 12.24 | 6 | 2108 | N   | ASN A 266 | 29.808 | 86.186 | 37.837 | 1.00 | 11.26 | 7 |
| 2067 | C   | GLY A 259 | 32.510 | 78.690 | 37.891 | 1.00 | 11.55 | 6 | 2109 | CA  | ASN A 266 | 28.739 | 85.402 | 37.199 | 1.00 | 12.93 | 6 |
| 2068 | O   | GLY A 259 | 31.417 | 78.276 | 38.227 | 1.00 | 12.61 | 8 | 2110 | C   | ASN A 266 | 28.140 | 84.338 | 38.110 | 1.00 | 13.52 | 6 |
| 2069 | N   | ASP A 260 | 32.921 | 79.963 | 37.891 | 1.00 | 11.45 | 7 | 2111 | O   | ASN A 266 | 27.364 | 83.484 | 37.632 | 1.00 | 11.82 | 8 |
| 2070 | CA  | ASP A 260 | 32.064 | 81.004 | 38.486 | 1.00 | 10.59 | 6 | 2112 | CB  | ASN A 266 | 29.289 | 84.792 | 35.855 | 1.00 | 15.03 | 6 |
| 2071 | C   | ASP A 260 | 31.718 | 80.614 | 39.947 | 1.00 | 12.08 | 6 | 2113 | CG  | ASN A 266 | 29.632 | 85.944 | 34.889 | 1.00 | 15.26 | 6 |
| 2072 | O   | ASP A 260 | 30.554 | 80.528 | 40.317 | 1.00 | 11.34 | 8 | 2114 | OD1 | ASN A 266 | 28.938 | 86.955 | 34.822 | 1.00 | 13.24 | 8 |
| 2073 | CB  | ASP A 260 | 30.792 | 81.286 | 37.665 | 1.00 | 13.01 | 6 | 2115 | ND2 | ASN A 266 | 30.698 | 85.797 | 34.146 | 1.00 | 14.64 | 7 |
| 2074 | CG  | ASP A 260 | 31.160 | 81.807 | 36.269 | 1.00 | 16.43 | 6 | 2116 | N   | HIS A 267 | 28.621 | 84.306 | 39.353 | 1.00 | 12.23 | 7 |
| 2075 | OD1 | ASP A 260 | 32.136 | 82.593 | 36.148 | 1.00 | 13.58 | 8 | 2117 | CA  | HIS A 267 | 28.106 | 83.276 | 40.271 | 1.00 | 13.10 | 6 |
| 2076 | OD2 | ASP A 260 | 30.486 | 81.502 | 35.274 | 1.00 | 14.47 | 8 | 2118 | C   | HIS A 267 | 26.596 | 83.276 | 40.469 | 1.00 | 13.44 | 6 |
| 2077 | N   | ASP A 261 | 32.812 | 80.528 | 40.708 | 1.00 | 10.89 | 7 | 2119 | O   | HIS A 267 | 25.999 | 82.182 | 40.399 | 1.00 | 12.11 | 8 |
| 2078 | CA  | ASP A 261 | 32.709 | 80.239 | 42.158 | 1.00 | 13.96 | 6 | 2120 | CB  | HIS A 267 | 28.852 | 83.439 | 41.616 | 1.00 | 10.82 | 6 |
| 2079 | C   | ASP A 261 | 32.059 | 81.369 | 42.936 | 1.00 | 12.00 | 6 | 2121 | CG  | HIS A 267 | 28.469 | 82.306 | 42.563 | 1.00 | 12.37 | 6 |
| 2080 | O   | ASP A 261 | 31.920 | 82.528 | 42.502 | 1.00 | 13.08 | 8 | 2122 | ND1 | HIS A 267 | 28.877 | 81.020 | 42.410 | 1.00 | 11.65 | 7 |
| 2081 | CB  | ASP A 261 | 34.125 | 79.875 | 42.610 | 1.00 | 17.34 | 6 | 2123 | CD2 | HIS A 267 | 27.637 | 82.360 | 43.640 | 1.00 | 15.29 | 6 |
| 2082 | CG  | ASP A 261 | 34.615 | 78.518 | 42.074 | 1.00 | 18.47 | 6 | 2124 | CE1 | HIS A 267 | 28.355 | 80.278 | 43.375 | 1.00 | 12.97 | 6 |
| 2083 | OD1 | ASP A 261 | 33.990 | 77.881 | 41.181 | 1.00 | 22.23 | 8 | 2125 | NE2 | HIS A 267 | 27.608 | 81.080 | 44.153 | 1.00 | 11.63 | 7 |
| 2084 | OD2 | ASP A 261 | 35.642 | 78.035 | 42.569 | 1.00 | 20.46 | 8 | 2126 | N   | LEU A 268 | 26.001 | 84.430 | 40.726 | 1.00 | 10.81 | 7 |
| 2085 | N   | PRO A 262 | 31.751 | 81.124 | 44.230 | 1.00 | 11.36 | 7 | 2127 | CA  | LEU A 268 | 24.548 | 84.455 | 40.988 | 1.00 | 13.40 | 6 |
| 2086 | CA  | PRO A 262 | 31.155 | 82.197 | 45.033 | 1.00 | 13.50 | 6 | 2128 | C   | LEU A 268 | 23.765 | 83.997 | 39.768 | 1.00 | 11.02 | 6 |
| 2087 | C   | PRO A 262 | 32.085 | 83.428 | 45.042 | 1.00 | 15.27 | 6 | 2129 | O   | LEU A 268 | 22.745 | 83.268 | 39.957 | 1.00 | 12.74 | 8 |
| 2088 | O   | PRO A 262 | 33.325 | 83.254 | 45.078 | 1.00 | 17.80 | 8 | 2130 | CB  | LEU A 268 | 24.169 | 85.889 | 41.374 | 1.00 | 14.95 | 6 |
| 2089 | CB  | PRO A 262 | 30.973 | 81.583 | 46.445 | 1.00 | 14.74 | 6 | 2131 | CG  | LEU A 268 | 22.599 | 86.052 | 41.471 | 1.00 | 19.99 | 6 |
| 2090 | CG  | PRO A 262 | 30.818 | 80.086 | 46.071 | 1.00 | 13.76 | 6 | 2132 | CD1 | LEU A 268 | 22.040 | 85.151 | 42.563 | 1.00 | 24.25 | 6 |
| 2091 | CD  | PRO A 262 | 31.873 | 79.856 | 44.938 | 1.00 | 11.66 | 6 | 2133 | CD2 | LEU A 268 | 22.298 | 87.536 | 41.677 | 1.00 | 25.18 | 6 |
| 2092 | N   | GLY A 263 | 31.385 | 84.560 | 45.069 | 1.00 | 20.11 | 7 | 2134 | N   | GLU A 269 | 24.210 | 84.274 | 38.549 | 1.00 | 11.51 | 7 |
| 2093 | CA  | GLY A 263 | 32.178 | 85.810 | 45.091 | 1.00 | 20.82 | 6 | 2135 | CA  | GLU A 269 | 23.495 | 83.760 | 37.381 | 1.00 | 11.81 | 6 |
| 2094 | C   | GLY A 263 | 32.444 | 86.343 | 43.693 | 1.00 | 22.93 | 6 | 2136 | C   | GLU A 269 | 23.525 | 82.221 | 37.386 | 1.00 | 10.11 | 6 |
| 2095 | O   | GLY A 263 | 33.030 | 87.433 | 43.565 | 1.00 | 26.12 | 8 | 2137 | O   | GLU A 269 | 22.512 | 81.596 | 37.067 | 1.00 | 11.07 | 8 |
| 2096 | N   | THR A 264 | 32.204 | 85.581 | 42.640 | 1.00 | 16.30 | 7 | 2138 | CB  | GLU A 269 | 24.190 | 84.360 | 36.122 | 1.00 | 13.26 | 6 |

2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2149 2150 2151 2152 2153 2154 2155 2156 2157 2158 2159 2160 2161 2162 2163 2164 2165 2166 2167 2168 2169 2170 2171 2172 2173 2174 2175 2176 2177 2178 2179 2180

|           |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|-----------|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| CG        | GLU A 269 | 23.490 | 83.803 | 34.867 | 1.00 | 11.45 | 6 | 2181 | OH  | TYR A 273 | 21.365 | 74.258 | 31.956 | 1.00 | 11.35 | 8 |
| CD        | GLU A 269 | 24.122 | 84.417 | 33.582 | 1.00 | 13.11 | 6 | 2182 | N   | ALA A 274 | 20.678 | 77.001 | 38.308 | 1.00 | 10.68 | 7 |
| OE1       | GLU A 269 | 24.906 | 85.369 | 33.643 | 1.00 | 12.92 | 8 | 2183 | CA  | ALA A 274 | 20.449 | 75.697 | 39.008 | 1.00 | 10.66 | 6 |
| OE2       | GLU A 269 | 23.720 | 83.906 | 32.525 | 1.00 | 12.17 | 8 | 2184 | C   | ALA A 274 | 19.062 | 75.725 | 39.677 | 1.00 | 10.79 | 6 |
| N         | LYS A 270 | 24.678 | 81.608 | 37.720 | 1.00 | 9.00  | 7 | 2185 | O   | ALA A 274 | 18.478 | 74.649 | 39.796 | 1.00 | 11.53 | 8 |
| CA        | LYS A 270 | 24.754 | 80.156 | 37.787 | 1.00 | 9.72  | 6 | 2186 | CB  | ALA A 274 | 21.539 | 75.560 | 40.092 | 1.00 | 12.82 | 6 |
| C         | LYS A 270 | 23.806 | 79.578 | 38.862 | 1.00 | 10.98 | 6 | 2187 | N   | ASN A 275 | 18.692 | 76.887 | 40.217 | 1.00 | 11.15 | 7 |
| O         | LYS A 270 | 23.079 | 78.613 | 38.609 | 1.00 | 10.64 | 8 | 2188 | CA  | ASN A 275 | 17.443 | 76.882 | 40.998 | 1.00 | 11.26 | 6 |
| CB        | LYS A 270 | 26.221 | 79.709 | 38.063 | 1.00 | 10.49 | 6 | 2189 | C   | ASN A 275 | 16.199 | 77.051 | 40.131 | 1.00 | 10.88 | 6 |
| CG        | LYS A 270 | 26.259 | 78.174 | 38.299 | 1.00 | 10.05 | 6 | 2190 | O   | ASN A 275 | 15.082 | 76.705 | 40.606 | 1.00 | 11.83 | 8 |
| LYS A 270 |           | 27.725 | 77.682 | 38.502 | 1.00 | 8.77  | 6 | 2191 | CB  | ASN A 275 | 17.490 | 78.056 | 42.004 | 1.00 | 11.31 | 6 |
| LYS A 270 |           | 28.236 | 78.181 | 39.869 | 1.00 | 9.57  | 6 | 2192 | CG  | ASN A 275 | 18.495 | 77.768 | 43.107 | 1.00 | 11.97 | 6 |
| LYS A 270 |           | 29.600 | 77.515 | 40.161 | 1.00 | 11.56 | 7 | 2193 | OD1 | ASN A 275 | 18.987 | 76.661 | 43.214 | 1.00 | 12.55 | 8 |
| NZ        | LYS A 270 | 23.765 | 80.218 | 40.038 | 1.00 | 11.90 | 7 | 2194 | ND2 | ASN A 275 | 18.759 | 78.816 | 43.934 | 1.00 | 12.55 | 7 |
| CA        | VAL A 271 | 22.847 | 79.712 | 41.105 | 1.00 | 10.97 | 6 | 2195 | N   | ASN A 276 | 16.322 | 77.453 | 38.842 | 1.00 | 11.20 | 7 |
| C         | VAL A 271 | 21.392 | 79.835 | 40.608 | 1.00 | 10.81 | 6 | 2196 | CA  | ASN A 276 | 15.129 | 77.705 | 38.045 | 1.00 | 12.25 | 6 |
| O         | VAL A 271 | 20.583 | 78.951 | 40.827 | 1.00 | 11.67 | 8 | 2197 | C   | ASN A 276 | 15.023 | 76.992 | 36.720 | 1.00 | 14.18 | 6 |
| CB        | VAL A 271 | 23.044 | 80.608 | 42.346 | 1.00 | 13.53 | 6 | 2198 | O   | ASN A 276 | 13.932 | 76.820 | 36.165 | 1.00 | 11.89 | 8 |
| CG1       | VAL A 271 | 22.016 | 80.248 | 43.435 | 1.00 | 12.11 | 6 | 2199 | CB  | ASN A 276 | 15.134 | 79.197 | 37.632 | 1.00 | 9.94  | 6 |
| CG2       | VAL A 271 | 24.455 | 80.307 | 42.888 | 1.00 | 12.46 | 6 | 2200 | CG  | ASN A 276 | 14.629 | 80.023 | 38.806 | 1.00 | 14.75 | 6 |
| N         | ARG A 272 | 21.064 | 80.978 | 39.983 | 1.00 | 11.20 | 7 | 2201 | OD1 | ASN A 276 | 13.365 | 80.089 | 38.826 | 1.00 | 16.83 | 8 |
| CA        | ARG A 272 | 19.668 | 81.127 | 39.458 | 1.00 | 11.53 | 6 | 2202 | ND2 | ASN A 276 | 15.551 | 80.529 | 39.612 | 1.00 | 16.12 | 7 |
| C         | ARG A 272 | 19.328 | 80.041 | 38.439 | 1.00 | 10.29 | 6 | 2203 | N   | SER A 277 | 16.151 | 76.504 | 36.173 | 1.00 | 10.52 | 7 |
| O         | ARG A 272 | 18.208 | 79.506 | 38.389 | 1.00 | 11.34 | 8 | 2204 | CA  | SER A 277 | 16.064 | 75.974 | 34.811 | 1.00 | 11.82 | 6 |
| CB        | ARG A 272 | 19.462 | 82.540 | 38.859 | 1.00 | 9.74  | 6 | 2205 | C   | SER A 277 | 15.497 | 74.585 | 34.678 | 1.00 | 11.16 | 6 |
| CG        | ARG A 272 | 19.220 | 83.552 | 40.027 | 1.00 | 11.97 | 6 | 2206 | O   | SER A 277 | 15.204 | 74.178 | 33.545 | 1.00 | 12.16 | 8 |
| CD        | ARG A 272 | 19.405 | 85.000 | 39.483 | 1.00 | 10.96 | 6 | 2207 | CB  | SER A 277 | 17.502 | 75.911 | 34.204 | 1.00 | 11.66 | 6 |
| NE        | ARG A 272 | 18.600 | 85.394 | 38.306 | 1.00 | 12.10 | 7 | 2208 | OG  | SER A 277 | 18.257 | 74.877 | 34.872 | 1.00 | 12.14 | 8 |
| CZ        | ARG A 272 | 17.297 | 85.759 | 38.377 | 1.00 | 14.61 | 6 | 2209 | N   | GLY A 278 | 15.371 | 73.851 | 35.795 | 1.00 | 11.36 | 7 |
| NH1       | ARG A 272 | 16.541 | 85.765 | 39.493 | 1.00 | 12.14 | 7 | 2210 | CA  | GLY A 278 | 15.051 | 72.411 | 35.697 | 1.00 | 11.40 | 6 |
| NH2       | ARG A 272 | 16.734 | 86.132 | 37.232 | 1.00 | 12.07 | 7 | 2211 | C   | GLY A 278 | 16.263 | 71.565 | 35.375 | 1.00 | 11.97 | 6 |
| N         | TYR A 273 | 20.329 | 79.790 | 37.553 | 1.00 | 10.33 | 7 | 2212 | O   | GLY A 278 | 16.115 | 70.348 | 35.279 | 1.00 | 13.61 | 8 |
| CA        | TYR A 273 | 20.116 | 78.669 | 36.589 | 1.00 | 11.57 | 6 | 2213 | N   | VAL A 279 | 17.442 | 72.180 | 35.342 | 1.00 | 12.14 | 7 |
| C         | TYR A 273 | 19.882 | 77.355 | 37.328 | 1.00 | 9.14  | 6 | 2214 | CA  | VAL A 279 | 18.673 | 71.427 | 35.090 | 1.00 | 10.48 | 6 |
| O         | TYR A 273 | 18.931 | 76.590 | 36.993 | 1.00 | 12.29 | 8 | 2215 | C   | VAL A 279 | 19.552 | 71.645 | 36.348 | 1.00 | 11.31 | 6 |
| CB        | TYR A 273 | 21.415 | 78.569 | 35.742 | 1.00 | 9.07  | 6 | 2216 | O   | VAL A 279 | 19.814 | 72.782 | 36.732 | 1.00 | 12.60 | 8 |
| CG        | TYR A 273 | 21.388 | 77.445 | 34.693 | 1.00 | 8.78  | 6 | 2217 | CB  | VAL A 279 | 19.362 | 71.989 | 33.830 | 1.00 | 11.56 | 6 |
| CD1       | TYR A 273 | 21.708 | 76.144 | 35.110 | 1.00 | 11.52 | 6 | 2218 | CG1 | VAL A 279 | 20.628 | 71.191 | 33.543 | 1.00 | 10.87 | 6 |
| CD2       | TYR A 273 | 21.054 | 77.630 | 33.363 | 1.00 | 9.55  | 6 | 2219 | CG2 | VAL A 279 | 18.429 | 71.824 | 32.592 | 1.00 | 13.38 | 6 |
| CE1       | TYR A 273 | 21.663 | 75.071 | 34.218 | 1.00 | 9.62  | 6 | 2220 | N   | ASN A 280 | 20.053 | 70.556 | 36.919 | 1.00 | 10.03 | 7 |
| CE2       | TYR A 273 | 21.087 | 76.577 | 32.482 | 1.00 | 8.45  | 6 | 2221 | CA  | ASN A 280 | 20.918 | 70.714 | 38.122 | 1.00 | 10.49 | 6 |
| CZ        | TYR A 273 | 21.366 | 75.301 | 32.885 | 1.00 | 10.47 | 6 | 2222 | C   | ASN A 280 | 22.294 | 71.095 | 37.572 | 1.00 | 13.05 | 6 |

|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2223 | O   | ASN A 280 | 22.506 | 71.116 | 36.365 | 1.00 | 12.57 | 8 | 2265 | O   | ASP A 285 | 33.806 | 75.092 | 45.468 | 1.00 | 11.00 | 8 |
| 2224 | CB  | ASN A 280 | 20.968 | 69.368 | 38.864 | 1.00 | 11.26 | 6 | 2266 | CB  | ASP A 285 | 30.773 | 76.068 | 44.545 | 1.00 | 9.55  | 6 |
| 2225 | CG  | ASN A 280 | 19.492 | 69.056 | 39.263 | 1.00 | 9.85  | 6 | 2267 | CG  | ASP A 285 | 29.979 | 77.042 | 43.692 | 1.00 | 10.92 | 6 |
| 2226 | OD1 | ASN A 280 | 18.839 | 69.805 | 39.990 | 1.00 | 10.91 | 8 | 2268 | OD1 | ASP A 285 | 30.499 | 77.631 | 42.710 | 1.00 | 12.04 | 8 |
| 2227 | ND2 | ASN A 280 | 18.974 | 67.913 | 38.787 | 1.00 | 10.65 | 7 | 2269 | OD2 | ASP A 285 | 28.773 | 77.214 | 44.043 | 1.00 | 12.59 | 8 |
| 2228 | N   | VAL A 281 | 23.262 | 71.312 | 38.492 | 1.00 | 11.45 | 7 | 2270 | N   | LEU A 286 | 32.248 | 73.464 | 45.128 | 1.00 | 10.30 | 7 |
| 2229 | CA  | VAL A 281 | 24.622 | 71.621 | 37.977 | 1.00 | 9.71  | 6 | 2271 | CA  | LEU A 286 | 32.959 | 72.569 | 46.061 | 1.00 | 9.08  | 6 |
| 2230 | C   | VAL A 281 | 25.671 | 70.782 | 38.660 | 1.00 | 11.24 | 6 | 2272 | C   | LEU A 286 | 34.219 | 71.940 | 45.505 | 1.00 | 9.26  | 6 |
| 2231 | O   | VAL A 281 | 25.581 | 70.318 | 39.799 | 1.00 | 11.15 | 8 | 2273 | O   | LEU A 286 | 35.179 | 71.757 | 46.238 | 1.00 | 11.04 | 8 |
| 2232 | CB  | VAL A 281 | 25.013 | 73.104 | 38.187 | 1.00 | 9.82  | 6 | 2274 | CB  | LEU A 286 | 31.968 | 71.419 | 46.481 | 1.00 | 9.12  | 6 |
| 2233 | CG1 | VAL A 281 | 24.019 | 74.024 | 37.397 | 1.00 | 10.47 | 6 | 2275 | CG  | LEU A 286 | 32.367 | 70.697 | 47.790 | 1.00 | 10.68 | 6 |
| 2234 | CG2 | VAL A 281 | 25.038 | 73.569 | 39.638 | 1.00 | 11.52 | 6 | 2276 | CD1 | LEU A 286 | 32.357 | 71.580 | 49.023 | 1.00 | 15.93 | 6 |
| 2235 | N   | LEU A 282 | 26.786 | 70.675 | 37.904 | 1.00 | 9.31  | 7 | 2277 | CD2 | LEU A 286 | 31.384 | 69.510 | 47.999 | 1.00 | 13.68 | 6 |
| 2236 | CA  | LEU A 282 | 28.031 | 70.087 | 38.460 | 1.00 | 10.27 | 6 | 2278 | N   | ASN A 287 | 34.226 | 71.683 | 44.168 | 1.00 | 9.32  | 7 |
| 2237 | C   | LEU A 282 | 28.631 | 71.063 | 39.476 | 1.00 | 11.17 | 6 | 2279 | CA  | ASN A 287 | 35.441 | 71.091 | 43.586 | 1.00 | 10.65 | 6 |
| 2238 | O   | LEU A 282 | 28.577 | 72.295 | 39.298 | 1.00 | 12.65 | 8 | 2280 | C   | ASN A 287 | 36.687 | 71.937 | 43.872 | 1.00 | 9.75  | 6 |
| 2239 | CB  | LEU A 282 | 29.022 | 69.883 | 37.283 | 1.00 | 10.13 | 6 | 2281 | O   | ASN A 287 | 37.751 | 71.401 | 44.184 | 1.00 | 10.35 | 8 |
| 2240 | CG  | LEU A 282 | 28.650 | 68.558 | 36.538 | 1.00 | 11.97 | 6 | 2282 | CB  | ASN A 287 | 35.269 | 71.000 | 42.039 | 1.00 | 8.74  | 6 |
| 2241 | CD1 | LEU A 282 | 29.159 | 68.726 | 35.102 | 1.00 | 16.51 | 6 | 2283 | CG  | ASN A 287 | 36.571 | 70.507 | 41.392 | 1.00 | 11.79 | 6 |
| 2242 | CD2 | LEU A 282 | 29.314 | 67.351 | 37.196 | 1.00 | 12.93 | 6 | 2284 | OD1 | ASN A 287 | 37.171 | 71.318 | 40.654 | 1.00 | 11.65 | 8 |
| 2243 | N   | ASP A 283 | 29.128 | 70.458 | 40.581 | 1.00 | 9.33  | 7 | 2285 | ND2 | ASN A 287 | 36.866 | 69.245 | 41.597 | 1.00 | 9.92  | 7 |
| 2244 | CA  | ASP A 283 | 29.503 | 71.304 | 41.764 | 1.00 | 11.76 | 6 | 2286 | N   | THR A 288 | 36.588 | 73.275 | 43.719 | 1.00 | 9.52  | 7 |
| 2245 | C   | ASP A 283 | 30.935 | 71.778 | 41.696 | 1.00 | 11.31 | 6 | 2287 | CA  | THR A 288 | 37.769 | 74.106 | 43.907 | 1.00 | 11.58 | 6 |
| 2246 | O   | ASP A 283 | 31.877 | 71.275 | 42.316 | 1.00 | 11.22 | 8 | 2288 | C   | THR A 288 | 38.367 | 73.906 | 45.292 | 1.00 | 10.74 | 6 |
| 2247 | CB  | ASP A 283 | 29.212 | 70.451 | 43.014 | 1.00 | 8.73  | 6 | 2289 | O   | THR A 288 | 39.593 | 73.741 | 45.486 | 1.00 | 13.25 | 8 |
| 2248 | CG  | ASP A 283 | 29.282 | 71.343 | 44.271 | 1.00 | 11.60 | 6 | 2290 | CB  | THR A 288 | 37.365 | 75.596 | 43.745 | 1.00 | 15.82 | 6 |
| 2249 | OD1 | ASP A 283 | 29.655 | 72.526 | 44.259 | 1.00 | 10.06 | 8 | 2291 | OG1 | THR A 288 | 36.906 | 75.753 | 42.397 | 1.00 | 16.55 | 8 |
| 2250 | OD2 | ASP A 283 | 28.866 | 70.758 | 45.290 | 1.00 | 11.95 | 8 | 2292 | CG2 | THR A 288 | 38.641 | 76.459 | 43.984 | 1.00 | 14.43 | 6 |
| 2251 | N   | PHE A 284 | 31.108 | 72.815 | 40.834 | 1.00 | 10.41 | 7 | 2293 | N   | VAL A 289 | 37.440 | 73.847 | 46.268 | 1.00 | 8.64  | 7 |
| 2252 | CA  | PHE A 284 | 32.439 | 73.424 | 40.731 | 1.00 | 10.33 | 6 | 2294 | CA  | VAL A 289 | 37.915 | 73.732 | 47.655 | 1.00 | 8.82  | 6 |
| 2253 | C   | PHE A 284 | 32.746 | 74.271 | 41.966 | 1.00 | 11.21 | 6 | 2295 | C   | VAL A 289 | 38.401 | 72.341 | 47.985 | 1.00 | 11.04 | 6 |
| 2254 | O   | PHE A 284 | 33.941 | 74.331 | 42.313 | 1.00 | 12.52 | 8 | 2296 | O   | VAL A 289 | 39.438 | 72.184 | 48.642 | 1.00 | 11.67 | 8 |
| 2255 | CB  | PHE A 284 | 32.509 | 74.409 | 39.517 | 1.00 | 10.51 | 6 | 2297 | CB  | VAL A 289 | 36.780 | 74.237 | 48.605 | 1.00 | 11.02 | 6 |
| 2256 | CG  | PHE A 284 | 32.750 | 73.575 | 38.227 | 1.00 | 10.01 | 6 | 2298 | CG1 | VAL A 289 | 37.297 | 74.258 | 50.051 | 1.00 | 10.38 | 6 |
| 2257 | CD1 | PHE A 284 | 31.725 | 72.991 | 37.520 | 1.00 | 11.07 | 6 | 2299 | CG2 | VAL A 289 | 36.323 | 75.632 | 48.191 | 1.00 | 11.61 | 6 |
| 2258 | CD2 | PHE A 284 | 34.073 | 73.416 | 37.765 | 1.00 | 11.57 | 6 | 2300 | N   | ILE A 290 | 37.764 | 71.287 | 47.430 | 1.00 | 9.86  | 7 |
| 2259 | CE1 | PHE A 284 | 31.925 | 72.232 | 36.386 | 1.00 | 12.29 | 6 | 2301 | CA  | ILE A 290 | 38.262 | 69.911 | 47.642 | 1.00 | 8.30  | 6 |
| 2260 | CE2 | PHE A 284 | 34.292 | 72.665 | 36.596 | 1.00 | 11.45 | 6 | 2302 | C   | ILE A 290 | 39.715 | 69.830 | 47.144 | 1.00 | 12.22 | 6 |
| 2261 | CZ  | PHE A 284 | 33.234 | 72.085 | 35.903 | 1.00 | 9.72  | 6 | 2303 | O   | ILE A 290 | 40.554 | 69.251 | 47.806 | 1.00 | 10.89 | 8 |
| 2262 | N   | ASP A 285 | 31.729 | 74.753 | 42.687 | 1.00 | 9.13  | 7 | 2304 | CB  | ILE A 290 | 37.342 | 68.979 | 46.851 | 1.00 | 9.93  | 6 |
| 2263 | CA  | ASP A 285 | 32.061 | 75.575 | 43.882 | 1.00 | 10.61 | 6 | 2305 | CG1 | ILE A 290 | 36.004 | 68.833 | 47.591 | 1.00 | 11.46 | 6 |
| 2264 | C   | ASP A 285 | 32.799 | 74.670 | 44.885 | 1.00 | 10.95 | 6 | 2306 | CG2 | ILE A 290 | 38.025 | 67.579 | 46.690 | 1.00 | 11.35 | 6 |

|      |     |     |   |     |        |        |        |      |       |   |      |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 2307 | CD1 | ILE | A | 290 | 34.964 | 68.108 | 46.700 | 1.00 | 11.71 | 6 | 2349 | N   | THR | A | 296 | 46.271 | 70.499 | 46.990 | 1.00 | 10.00 | 7 |
| 2308 | N   | ARG | A | 291 | 39.969 | 70.386 | 45.940 | 1.00 | 11.21 | 7 | 2350 | CA  | THR | A | 296 | 47.441 | 71.394 | 47.123 | 1.00 | 11.19 | 6 |
| 2309 | CA  | ARG | A | 291 | 41.352 | 70.246 | 45.455 | 1.00 | 10.67 | 6 | 2351 | C   | THR | A | 296 | 47.675 | 71.894 | 48.549 | 1.00 | 13.50 | 6 |
| 2310 | C   | ARG | A | 291 | 42.343 | 71.071 | 46.293 | 1.00 | 9.59  | 6 | 2352 | O   | THR | A | 296 | 48.755 | 72.436 | 48.874 | 1.00 | 12.22 | 8 |
| 2311 | O   | ARG | A | 291 | 43.481 | 70.627 | 46.380 | 1.00 | 12.39 | 8 | 2353 | CB  | THR | A | 296 | 47.162 | 72.647 | 46.253 | 1.00 | 11.65 | 6 |
| 2312 | CB  | ARG | A | 291 | 41.308 | 70.770 | 43.991 | 1.00 | 10.96 | 6 | 2354 | OG1 | THR | A | 296 | 46.005 | 73.276 | 46.812 | 1.00 | 15.42 | 8 |
| 2313 | CG  | ARG | A | 291 | 40.602 | 69.717 | 43.110 | 1.00 | 11.39 | 6 | 2355 | CG2 | THR | A | 296 | 46.976 | 72.308 | 44.770 | 1.00 | 13.16 | 6 |
| 2314 | CD  | ARG | A | 291 | 40.480 | 70.173 | 41.647 | 1.00 | 11.11 | 6 | 2356 | N   | PHE | A | 297 | 46.760 | 71.647 | 49.472 | 1.00 | 11.24 | 7 |
| 2315 | NE  | ARG | A | 291 | 41.729 | 70.343 | 40.907 | 1.00 | 11.15 | 7 | 2357 | CA  | PHE | A | 297 | 47.104 | 73.543 | 50.984 | 1.00 | 17.18 | 6 |
| 2316 | CZ  | ARG | A | 291 | 42.225 | 69.361 | 40.109 | 1.00 | 12.12 | 6 | 2358 | C   | PHE | A | 297 | 47.719 | 74.035 | 51.952 | 1.00 | 17.61 | 8 |
| 2317 | NH1 | ARG | A | 291 | 41.706 | 68.126 | 40.068 | 1.00 | 11.32 | 7 | 2359 | O   | PHE | A | 297 | 48.052 | 71.271 | 51.610 | 1.00 | 11.80 | 6 |
| 2318 | NH2 | ARG | A | 291 | 43.322 | 69.593 | 39.363 | 1.00 | 12.38 | 7 | 2360 | CB  | PHE | A | 297 | 47.630 | 69.924 | 52.199 | 1.00 | 14.38 | 6 |
| 2319 | N   | ASN | A | 292 | 41.972 | 72.204 | 46.801 | 1.00 | 12.65 | 7 | 2361 | CG  | PHE | A | 297 | 47.153 | 68.917 | 51.385 | 1.00 | 13.09 | 6 |
| 2320 | CA  | ASN | A | 292 | 42.894 | 73.001 | 47.653 | 1.00 | 11.32 | 6 | 2362 | CD1 | PHE | A | 297 | 47.760 | 69.711 | 53.565 | 1.00 | 11.70 | 6 |
| 2321 | C   | ASN | A | 292 | 42.983 | 72.376 | 49.051 | 1.00 | 11.68 | 6 | 2363 | CD2 | PHE | A | 297 | 46.821 | 67.656 | 51.854 | 1.00 | 12.95 | 6 |
| 2322 | O   | ASN | A | 292 | 44.074 | 72.565 | 49.634 | 1.00 | 11.50 | 8 | 2364 | CE1 | PHE | A | 297 | 47.438 | 68.444 | 54.064 | 1.00 | 12.92 | 6 |
| 2323 | CB  | ASN | A | 292 | 42.408 | 74.471 | 47.750 | 1.00 | 11.01 | 6 | 2365 | CE2 | PHE | A | 297 | 46.948 | 67.450 | 53.231 | 1.00 | 11.87 | 6 |
| 2324 | CG  | ASN | A | 292 | 42.593 | 75.238 | 46.379 | 1.00 | 14.57 | 6 | 2366 | CZ  | PHE | A | 297 | 46.411 | 74.322 | 50.183 | 1.00 | 13.51 | 7 |
| 2325 | OD1 | ASN | A | 292 | 43.466 | 74.831 | 45.665 | 1.00 | 19.84 | 8 | 2367 | N   | THR | A | 298 | 46.398 | 75.773 | 50.270 | 1.00 | 13.52 | 6 |
| 2326 | ND2 | ASN | A | 292 | 41.735 | 76.242 | 46.267 | 1.00 | 18.55 | 7 | 2368 | CA  | THR | A | 298 | 45.131 | 76.303 | 50.925 | 1.00 | 13.29 | 6 |
| 2327 | N   | VAL | A | 293 | 42.009 | 71.574 | 49.542 | 1.00 | 10.40 | 7 | 2369 | C   | THR | A | 298 | 45.018 | 77.505 | 51.220 | 1.00 | 15.14 | 8 |
| 2328 | CA  | VAL | A | 293 | 42.157 | 71.075 | 50.940 | 1.00 | 10.24 | 6 | 2370 | O   | THR | A | 298 | 46.488 | 76.437 | 48.870 | 1.00 | 13.68 | 8 |
| 2329 | C   | VAL | A | 293 | 42.861 | 69.743 | 50.969 | 1.00 | 11.21 | 6 | 2371 | CB  | THR | A | 298 | 45.446 | 75.982 | 48.035 | 1.00 | 12.95 | 6 |
| 2330 | O   | VAL | A | 293 | 43.748 | 69.520 | 51.783 | 1.00 | 11.98 | 8 | 2372 | OG1 | THR | A | 298 | 47.869 | 76.059 | 48.250 | 1.00 | 15.45 | 6 |
| 2331 | CB  | VAL | A | 293 | 40.703 | 70.961 | 51.499 | 1.00 | 10.95 | 6 | 2373 | CG2 | THR | A | 298 | 44.162 | 75.400 | 51.194 | 1.00 | 10.17 | 7 |
| 2332 | CG1 | VAL | A | 293 | 40.707 | 70.175 | 52.820 | 1.00 | 12.97 | 6 | 2374 | N   | GLN | A | 299 | 43.009 | 75.785 | 51.975 | 1.00 | 13.00 | 6 |
| 2333 | CG2 | VAL | A | 293 | 40.153 | 72.364 | 51.736 | 1.00 | 13.88 | 6 | 2375 | CA  | GLN | A | 299 | 42.852 | 74.738 | 53.114 | 1.00 | 14.72 | 6 |
| 2334 | N   | PHE | A | 294 | 42.479 | 68.858 | 50.033 | 1.00 | 11.12 | 7 | 2376 | C   | GLN | A | 299 | 43.624 | 73.753 | 53.094 | 1.00 | 14.92 | 8 |
| 2335 | CA  | PHE | A | 294 | 43.106 | 67.537 | 49.960 | 1.00 | 11.38 | 6 | 2377 | O   | GLN | A | 299 | 41.654 | 75.808 | 51.214 | 1.00 | 11.79 | 6 |
| 2336 | C   | PHE | A | 294 | 44.255 | 67.464 | 48.964 | 1.00 | 11.51 | 6 | 2378 | CB  | GLN | A | 299 | 41.692 | 77.072 | 50.299 | 1.00 | 14.80 | 6 |
| 2337 | O   | PHE | A | 294 | 45.095 | 66.540 | 49.093 | 1.00 | 11.86 | 8 | 2379 | CG  | GLN | A | 299 | 40.301 | 77.320 | 49.668 | 1.00 | 16.23 | 6 |
| 2338 | CB  | PHE | A | 294 | 42.063 | 66.455 | 49.553 | 1.00 | 11.70 | 6 | 2380 | CD  | GLN | A | 299 | 39.959 | 76.525 | 48.827 | 1.00 | 15.11 | 8 |
| 2339 | CG  | PHE | A | 294 | 40.936 | 66.334 | 50.584 | 1.00 | 11.57 | 6 | 2381 | OE1 | GLN | A | 299 | 39.635 | 78.376 | 50.107 | 1.00 | 17.75 | 7 |
| 2340 | CD1 | PHE | A | 294 | 41.178 | 65.683 | 51.808 | 1.00 | 11.48 | 6 | 2382 | NE2 | GLN | A | 299 | 42.031 | 75.020 | 54.106 | 1.00 | 13.71 | 7 |
| 2341 | CD2 | PHE | A | 294 | 39.707 | 66.865 | 50.295 | 1.00 | 13.60 | 6 | 2383 | N   | THR | A | 300 | 41.924 | 74.106 | 55.252 | 1.00 | 11.61 | 6 |
| 2342 | CE1 | PHE | A | 294 | 40.133 | 65.579 | 52.724 | 1.00 | 12.41 | 6 | 2384 | CA  | THR | A | 300 | 40.518 | 73.485 | 55.355 | 1.00 | 14.08 | 6 |
| 2343 | CE2 | PHE | A | 294 | 38.662 | 66.762 | 51.232 | 1.00 | 13.36 | 6 | 2385 | C   | THR | A | 300 | 39.580 | 73.874 | 54.644 | 1.00 | 11.91 | 8 |
| 2344 | CZ  | PHE | A | 294 | 38.880 | 66.104 | 52.463 | 1.00 | 13.22 | 6 | 2386 | O   | THR | A | 300 | 42.152 | 74.850 | 56.601 | 1.00 | 15.34 | 6 |
| 2345 | N   | GLY | A | 295 | 44.295 | 68.355 | 47.976 | 1.00 | 11.76 | 7 | 2387 | CB  | THR | A | 300 | 41.116 | 75.771 | 56.804 | 1.00 | 15.70 | 8 |
| 2346 | CA  | GLY | A | 295 | 45.328 | 68.234 | 46.907 | 1.00 | 12.36 | 6 | 2388 | OG1 | THR | A | 300 | 43.511 | 75.587 | 56.464 | 1.00 | 16.98 | 6 |
| 2347 | C   | GLY | A | 295 | 46.504 | 69.187 | 47.187 | 1.00 | 10.85 | 6 | 2389 | CG2 | THR | A | 300 | 40.337 | 72.672 | 56.443 | 1.00 | 11.88 | 7 |
| 2348 | O   | GLY | A | 295 | 47.547 | 68.676 | 47.612 | 1.00 | 13.29 | 8 |      |     |     |   |     |        |        |        |      |       |   |

|      |     |           |        |        |        |      |       |    |      |     |            |        |        |        |      |       |    |
|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|------------|--------|--------|--------|------|-------|----|
| 2391 | CA  | MET A 301 | 38.977 | 72.123 | 56.650 | 1.00 | 12.22 | 6  | 2433 | ND2 | ASN A 305  | 31.910 | 74.651 | 58.967 | 1.00 | 17.24 | 7  |
| 2392 | C   | MET A 301 | 37.972 | 73.216 | 56.994 | 1.00 | 12.44 | 6  | 2434 | N   | ASN A 306  | 33.061 | 75.772 | 55.272 | 1.00 | 11.86 | 7  |
| 2393 | O   | MET A 301 | 36.791 | 73.075 | 56.691 | 1.00 | 11.03 | 8  | 2435 | CA  | ASN A 306  | 32.418 | 77.036 | 54.848 | 1.00 | 12.68 | 6  |
| 2394 | CB  | MET A 301 | 38.935 | 71.065 | 57.800 | 1.00 | 12.80 | 6  | 2436 | C   | ASN A 306  | 31.740 | 76.830 | 53.499 | 1.00 | 13.44 | 6  |
| 2395 | CG  | MET A 301 | 39.707 | 69.787 | 57.393 | 1.00 | 11.05 | 6  | 2437 | O   | ASN A 306  | 30.672 | 77.409 | 53.225 | 1.00 | 13.40 | 8  |
| 2396 | SD  | MET A 301 | 39.027 | 69.014 | 55.895 | 1.00 | 12.28 | 16 | 2438 | CB  | ASN A 306  | 33.438 | 78.176 | 54.774 | 1.00 | 12.13 | 6  |
| 2397 | CE  | MET A 301 | 39.724 | 67.366 | 56.047 | 1.00 | 14.34 | 6  | 2439 | CG  | ASN A 306  | 33.863 | 78.686 | 56.143 | 1.00 | 20.79 | 6  |
| 2398 | N   | TYR A 302 | 38.408 | 74.374 | 57.555 | 1.00 | 12.00 | 7  | 2440 | OD1 | ASN A 306  | 33.275 | 78.499 | 57.233 | 1.00 | 23.19 | 8  |
| 2399 | CA  | TYR A 302 | 37.462 | 75.453 | 57.759 | 1.00 | 10.79 | 6  | 2441 | ND2 | ASN A 306  | 34.959 | 79.477 | 56.155 | 1.00 | 24.17 | 7  |
| 2400 | C   | TYR A 302 | 36.898 | 75.974 | 56.430 | 1.00 | 11.89 | 6  | 2442 | N   | MET A 307  | 32.405 | 76.105 | 52.589 | 1.00 | 11.55 | 7  |
| 2401 | O   | TYR A 302 | 35.694 | 76.181 | 56.325 | 1.00 | 12.65 | 8  | 2443 | CA  | MET A 307  | 31.750 | 75.915 | 51.254 | 1.00 | 11.38 | 6  |
| 2402 | CB  | TYR A 302 | 38.131 | 76.626 | 58.505 | 1.00 | 10.20 | 6  | 2444 | C   | MET A 307  | 30.590 | 74.957 | 51.272 | 1.00 | 12.48 | 6  |
| 2403 | CG  | TYR A 302 | 38.409 | 76.271 | 59.983 | 1.00 | 11.51 | 6  | 2445 | O   | MET A 307  | 29.639 | 75.156 | 50.512 | 1.00 | 13.10 | 8  |
| 2404 | CD1 | TYR A 302 | 37.375 | 76.197 | 60.914 | 1.00 | 16.19 | 6  | 2446 | CB  | MET A 307  | 32.849 | 75.431 | 50.252 | 1.00 | 12.11 | 6  |
| 2405 | CD2 | TYR A 302 | 39.739 | 76.057 | 60.344 | 1.00 | 17.97 | 6  | 2447 | CG  | MET A 307  | 32.375 | 75.462 | 48.767 | 1.00 | 12.14 | 6  |
| 2406 | CE1 | TYR A 302 | 37.736 | 75.884 | 62.236 | 1.00 | 18.06 | 6  | 2448 | SD  | MET A 307  | 31.759 | 77.075 | 48.246 | 1.00 | 12.77 | 16 |
| 2407 | CE2 | TYR A 302 | 40.062 | 75.723 | 61.683 | 1.00 | 15.93 | 6  | 2449 | CE  | MET A 307  | 33.282 | 78.010 | 48.324 | 1.00 | 13.86 | 6  |
| 2408 | CZ  | TYR A 302 | 39.029 | 75.670 | 62.567 | 1.00 | 19.00 | 6  | 2450 | N   | VAL A 308  | 30.592 | 73.951 | 52.152 | 1.00 | 10.38 | 7  |
| 2409 | OH  | TYR A 302 | 39.409 | 75.355 | 63.905 | 1.00 | 21.46 | 8  | 2451 | CA  | VAL A 308  | 29.383 | 73.136 | 52.340 | 1.00 | 10.10 | 6  |
| 2410 | N   | ASP A 303 | 37.763 | 76.026 | 55.418 | 1.00 | 13.06 | 7  | 2452 | C   | VAL A 308  | 28.272 | 74.049 | 52.822 | 1.00 | 11.64 | 6  |
| 2411 | CA  | ASP A 303 | 37.256 | 76.434 | 54.104 | 1.00 | 12.54 | 6  | 2453 | O   | VAL A 308  | 27.153 | 73.974 | 52.321 | 1.00 | 13.14 | 8  |
| 2412 | C   | ASP A 303 | 36.285 | 75.409 | 53.492 | 1.00 | 11.88 | 6  | 2454 | CB  | VAL A 308  | 29.712 | 72.052 | 53.406 | 1.00 | 13.16 | 6  |
| 2413 | O   | ASP A 303 | 35.330 | 75.782 | 52.785 | 1.00 | 13.46 | 8  | 2455 | CG1 | VAL A 308  | 28.388 | 71.356 | 53.770 | 1.00 | 14.05 | 6  |
| 2414 | CB  | ASP A 303 | 38.419 | 76.666 | 53.133 | 1.00 | 10.93 | 6  | 2456 | CG2 | VAL A 308  | 30.641 | 71.038 | 52.727 | 1.00 | 13.08 | 6  |
| 2415 | CG  | ASP A 303 | 39.386 | 77.734 | 53.654 | 1.00 | 14.78 | 6  | 2457 | N   | ASN A 309  | 28.541 | 74.952 | 53.784 | 1.00 | 12.04 | 7  |
| 2416 | OD1 | ASP A 303 | 38.879 | 78.877 | 53.849 | 1.00 | 13.77 | 8  | 2458 | CA  | ASN A 309  | 27.479 | 75.848 | 54.264 | 1.00 | 12.56 | 6  |
| 2417 | OD2 | ASP A 303 | 40.573 | 77.435 | 53.832 | 1.00 | 13.10 | 8  | 2459 | C   | ASN A 309  | 27.073 | 76.824 | 53.176 | 1.00 | 13.56 | 6  |
| 2418 | N   | LEU A 304 | 36.602 | 74.152 | 53.720 | 1.00 | 11.36 | 7  | 2460 | O   | ASN A 309  | 25.875 | 77.017 | 53.030 | 1.00 | 15.38 | 8  |
| 2419 | CA  | LEU A 304 | 35.713 | 73.086 | 53.156 | 1.00 | 11.06 | 6  | 2461 | CB  | ASN A 309  | 27.997 | 76.680 | 55.470 | 1.00 | 14.00 | 6  |
| 2420 | C   | LEU A 304 | 34.348 | 73.181 | 53.841 | 1.00 | 12.95 | 6  | 2462 | CG  | ASN A 309  | 28.109 | 75.761 | 56.684 | 1.00 | 20.56 | 6  |
| 2421 | O   | LEU A 304 | 33.315 | 73.111 | 53.155 | 1.00 | 11.60 | 8  | 2463 | OD1 | ASN A 309  | 27.432 | 74.725 | 56.748 | 1.00 | 26.71 | 8  |
| 2422 | CB  | LEU A 304 | 36.393 | 71.742 | 53.367 | 1.00 | 10.48 | 6  | 2464 | ND2 | ASN A 309  | 28.967 | 76.208 | 57.595 | 1.00 | 21.18 | 7  |
| 2423 | CG  | LEU A 304 | 35.687 | 70.566 | 52.633 | 1.00 | 11.09 | 6  | 2465 | N   | GILN A 310 | 27.970 | 77.423 | 52.426 | 1.00 | 14.28 | 7  |
| 2424 | CD1 | LEU A 304 | 35.737 | 70.797 | 51.112 | 1.00 | 12.57 | 6  | 2466 | CA  | GILN A 310 | 27.549 | 78.422 | 51.422 | 1.00 | 13.95 | 6  |
| 2425 | CD2 | LEU A 304 | 36.397 | 69.248 | 52.971 | 1.00 | 12.54 | 6  | 2467 | C   | GILN A 310 | 26.734 | 77.754 | 50.319 | 1.00 | 13.50 | 6  |
| 2426 | N   | ASN A 305 | 34.290 | 73.255 | 55.180 | 1.00 | 11.76 | 7  | 2468 | O   | GILN A 310 | 25.672 | 78.286 | 49.942 | 1.00 | 14.03 | 8  |
| 2427 | CA  | ASN A 305 | 32.999 | 73.422 | 55.887 | 1.00 | 12.74 | 6  | 2469 | CB  | GILN A 310 | 28.821 | 79.123 | 50.869 | 1.00 | 14.99 | 6  |
| 2428 | C   | ASN A 305 | 32.308 | 74.720 | 55.479 | 1.00 | 11.54 | 6  | 2470 | CG  | GILN A 310 | 28.507 | 80.214 | 49.859 | 1.00 | 21.08 | 6  |
| 2429 | O   | ASN A 305 | 31.100 | 74.673 | 55.259 | 1.00 | 13.50 | 8  | 2471 | CD  | GILN A 310 | 29.734 | 81.169 | 49.819 | 1.00 | 21.08 | 6  |
| 2430 | CB  | ASN A 305 | 33.331 | 73.448 | 57.405 | 1.00 | 12.22 | 6  | 2472 | OE1 | GILN A 310 | 30.875 | 80.762 | 50.019 | 1.00 | 25.61 | 8  |
| 2431 | CG  | ASN A 305 | 32.014 | 73.551 | 58.210 | 1.00 | 12.84 | 6  | 2473 | NE2 | GILN A 310 | 29.417 | 82.401 | 49.600 | 1.00 | 25.23 | 7  |
| 2432 | OD1 | ASN A 305 | 31.174 | 72.669 | 58.097 | 1.00 | 13.98 | 8  | 2474 | N   | THR A 311  | 27.238 | 76.630 | 49.792 | 1.00 | 11.65 | 7  |

|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2475 | CA  | THR A 311 | 26.432 | 75.983 | 48.711 | 1.00 | 11.52 | 6 | 2517 | O   | LYS A 316 | 17.175 | 72.963 | 47.475 | 1.00 | 14.60 | 8 |
| 2476 | C   | THR A 311 | 25.089 | 75.459 | 49.257 | 1.00 | 12.57 | 6 | 2518 | CB  | LYS A 316 | 16.496 | 75.595 | 45.485 | 1.00 | 14.77 | 6 |
| 2477 | O   | THR A 311 | 24.039 | 75.572 | 48.599 | 1.00 | 13.81 | 8 | 2519 | CG  | LYS A 316 | 15.139 | 75.068 | 46.091 | 1.00 | 18.12 | 6 |
| 2478 | CB  | THR A 311 | 27.143 | 74.754 | 48.142 | 1.00 | 12.52 | 6 | 2520 | CD  | LYS A 316 | 13.982 | 75.856 | 45.565 | 1.00 | 22.24 | 6 |
| 2479 | OG1 | THR A 311 | 27.593 | 73.909 | 49.194 | 1.00 | 13.67 | 8 | 2521 | CE  | LYS A 316 | 12.683 | 75.166 | 46.061 | 1.00 | 19.23 | 6 |
| 2480 | CG2 | THR A 311 | 28.426 | 75.250 | 47.375 | 1.00 | 14.32 | 6 | 2522 | NZ  | LYS A 316 | 12.432 | 75.635 | 47.468 | 1.00 | 22.20 | 7 |
| 2481 | N   | GLY A 312 | 25.096 | 75.107 | 50.561 | 1.00 | 11.69 | 7 | 2523 | N   | TYR A 317 | 18.227 | 72.953 | 45.457 | 1.00 | 13.10 | 7 |
| 2482 | CA  | GLY A 312 | 23.812 | 74.642 | 51.137 | 1.00 | 14.78 | 6 | 2524 | CA  | TYR A 317 | 18.316 | 71.483 | 45.445 | 1.00 | 11.39 | 6 |
| 2483 | C   | GLY A 312 | 22.800 | 75.792 | 51.223 | 1.00 | 14.32 | 6 | 2525 | C   | TYR A 317 | 19.805 | 71.123 | 45.506 | 1.00 | 10.31 | 6 |
| 2484 | O   | GLY A 312 | 21.573 | 75.473 | 51.276 | 1.00 | 16.33 | 8 | 2526 | O   | TYR A 317 | 20.410 | 70.491 | 44.637 | 1.00 | 12.52 | 8 |
| 2485 | N   | ASN A 313 | 23.320 | 76.998 | 51.476 | 1.00 | 13.08 | 7 | 2527 | CB  | TYR A 317 | 17.652 | 70.893 | 44.157 | 1.00 | 12.53 | 6 |
| 2486 | CA  | ASN A 313 | 22.392 | 78.108 | 51.535 | 1.00 | 13.20 | 6 | 2528 | CG  | TYR A 317 | 16.221 | 71.387 | 44.004 | 1.00 | 13.61 | 6 |
| 2487 | C   | ASN A 313 | 21.980 | 78.575 | 50.150 | 1.00 | 14.89 | 6 | 2529 | CD1 | TYR A 317 | 15.272 | 70.932 | 44.915 | 1.00 | 14.65 | 6 |
| 2488 | O   | ASN A 313 | 20.827 | 79.097 | 50.014 | 1.00 | 20.75 | 8 | 2530 | CD2 | TYR A 317 | 15.800 | 72.280 | 43.030 | 1.00 | 14.34 | 6 |
| 2489 | CB  | ASN A 313 | 23.155 | 79.260 | 52.204 | 1.00 | 19.18 | 6 | 2531 | CE1 | TYR A 317 | 13.938 | 71.366 | 44.811 | 1.00 | 13.78 | 6 |
| 2490 | CG  | ASN A 313 | 23.210 | 79.024 | 53.718 | 1.00 | 30.91 | 6 | 2532 | CE2 | TYR A 317 | 14.511 | 72.767 | 42.890 | 1.00 | 12.10 | 6 |
| 2491 | OD1 | ASN A 313 | 22.384 | 78.310 | 54.281 | 1.00 | 30.04 | 8 | 2533 | CZ  | TYR A 317 | 13.604 | 72.246 | 43.832 | 1.00 | 15.19 | 6 |
| 2492 | ND2 | ASN A 313 | 24.152 | 79.691 | 54.360 | 1.00 | 31.03 | 7 | 2534 | OH  | TYR A 317 | 12.275 | 72.682 | 43.733 | 1.00 | 14.53 | 8 |
| 2493 | N   | GLU A 314 | 22.802 | 78.394 | 49.111 | 1.00 | 12.83 | 7 | 2535 | N   | LYS A 318 | 20.375 | 71.463 | 46.702 | 1.00 | 11.46 | 7 |
| 2494 | CA  | GLU A 314 | 22.396 | 79.060 | 47.822 | 1.00 | 11.95 | 6 | 2536 | CA  | LYS A 318 | 21.821 | 71.130 | 46.865 | 1.00 | 10.64 | 6 |
| 2495 | C   | GLU A 314 | 21.621 | 78.137 | 46.889 | 1.00 | 13.20 | 6 | 2537 | C   | LYS A 318 | 22.053 | 69.651 | 46.865 | 1.00 | 10.21 | 6 |
| 2496 | O   | GLU A 314 | 20.733 | 78.689 | 46.175 | 1.00 | 13.02 | 8 | 2538 | O   | LYS A 318 | 23.133 | 69.145 | 46.529 | 1.00 | 10.36 | 8 |
| 2497 | CB  | GLU A 314 | 23.753 | 79.394 | 47.117 | 1.00 | 10.17 | 6 | 2539 | CB  | LYS A 318 | 22.408 | 71.772 | 48.141 | 1.00 | 9.85  | 6 |
| 2498 | CG  | GLU A 314 | 24.503 | 80.510 | 47.842 | 1.00 | 12.02 | 6 | 2540 | CG  | LYS A 318 | 21.843 | 71.211 | 49.451 | 1.00 | 13.57 | 6 |
| 2499 | CD  | GLU A 314 | 25.715 | 80.987 | 46.985 | 1.00 | 15.94 | 6 | 2541 | CD  | LYS A 318 | 20.619 | 72.105 | 49.820 | 1.00 | 19.29 | 6 |
| 2500 | OE1 | GLU A 314 | 26.285 | 80.206 | 46.232 | 1.00 | 15.22 | 8 | 2542 | CE  | LYS A 318 | 20.309 | 72.064 | 51.345 | 1.00 | 19.13 | 6 |
| 2501 | OE2 | GLU A 314 | 26.164 | 82.100 | 47.284 | 1.00 | 24.00 | 8 | 2543 | NZ  | LYS A 318 | 19.066 | 72.819 | 51.636 | 1.00 | 20.57 | 7 |
| 2502 | N   | TYR A 315 | 21.992 | 76.840 | 46.892 | 1.00 | 11.76 | 7 | 2544 | N   | GLU A 319 | 21.044 | 68.796 | 47.174 | 1.00 | 9.32  | 7 |
| 2503 | CA  | TYR A 315 | 21.297 | 75.979 | 45.885 | 1.00 | 10.85 | 6 | 2545 | CA  | GLU A 319 | 21.217 | 67.359 | 47.096 | 1.00 | 11.07 | 6 |
| 2504 | C   | TYR A 315 | 20.032 | 75.368 | 46.506 | 1.00 | 12.73 | 6 | 2546 | C   | GLU A 319 | 21.164 | 66.802 | 45.667 | 1.00 | 12.26 | 6 |
| 2505 | O   | TYR A 315 | 20.140 | 74.648 | 47.510 | 1.00 | 12.47 | 8 | 2547 | O   | GLU A 319 | 21.469 | 65.627 | 45.504 | 1.00 | 11.85 | 8 |
| 2506 | CB  | TYR A 315 | 22.265 | 74.838 | 45.494 | 1.00 | 12.39 | 6 | 2548 | CB  | GLU A 319 | 20.021 | 66.636 | 47.827 | 1.00 | 12.74 | 6 |
| 2507 | CG  | TYR A 315 | 23.437 | 75.394 | 44.699 | 1.00 | 10.41 | 6 | 2549 | CG  | GLU A 319 | 19.998 | 67.027 | 49.320 | 1.00 | 15.35 | 6 |
| 2508 | CD1 | TYR A 315 | 23.270 | 75.610 | 43.316 | 1.00 | 11.23 | 6 | 2550 | CD  | GLU A 319 | 19.346 | 68.353 | 49.656 | 1.00 | 19.53 | 6 |
| 2509 | CD2 | TYR A 315 | 24.613 | 75.785 | 45.297 | 1.00 | 12.52 | 6 | 2551 | OE1 | GLU A 319 | 18.645 | 68.996 | 48.818 | 1.00 | 14.20 | 8 |
| 2510 | CE1 | TYR A 315 | 24.333 | 76.166 | 42.586 | 1.00 | 12.92 | 6 | 2552 | OE2 | GLU A 319 | 19.503 | 68.829 | 50.839 | 1.00 | 14.17 | 8 |
| 2511 | CE2 | TYR A 315 | 25.686 | 76.350 | 44.563 | 1.00 | 10.90 | 6 | 2553 | N   | ASN A 320 | 21.033 | 67.681 | 44.664 | 1.00 | 9.38  | 7 |
| 2512 | CZ  | TYR A 315 | 25.510 | 76.507 | 43.187 | 1.00 | 12.76 | 6 | 2554 | CA  | ASN A 320 | 21.155 | 67.324 | 43.285 | 1.00 | 9.77  | 6 |
| 2513 | OH  | TYR A 315 | 26.595 | 77.056 | 42.517 | 1.00 | 13.74 | 8 | 2555 | C   | ASN A 320 | 22.454 | 67.819 | 42.636 | 1.00 | 12.36 | 6 |
| 2514 | N   | LYS A 316 | 18.595 | 75.634 | 45.861 | 1.00 | 11.54 | 7 | 2556 | O   | ASN A 320 | 22.736 | 67.591 | 41.442 | 1.00 | 10.93 | 8 |
| 2515 | CA  | LYS A 316 | 17.638 | 75.080 | 46.395 | 1.00 | 14.39 | 6 | 2557 | CB  | ASN A 320 | 19.995 | 67.901 | 42.402 | 1.00 | 10.57 | 6 |
| 2516 | C   | LYS A 316 | 17.578 | 73.555 | 46.454 | 1.00 | 15.27 | 6 | 2558 | CG  | ASN A 320 | 18.660 | 67.290 | 42.784 | 1.00 | 14.03 | 6 |

|      |               |        |        |        |      |       |   |      |               |        |        |        |      |       |   |
|------|---------------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 2559 | OD1 ASN A 320 | 18.619 | 66.275 | 43.445 | 1.00 | 13.17 | 8 | 2601 | CG2AILE A 325 | 37.288 | 64.325 | 44.695 | 0.60 | 12.60 | 6 |
| 2560 | ND2 ASN A 320 | 17.558 | 67.901 | 42.323 | 1.00 | 10.64 | 7 | 2602 | CDIAILE A 325 | 39.550 | 62.693 | 43.585 | 0.60 | 10.36 | 6 |
| 2561 | N LEU A 321   | 23.285 | 68.499 | 43.422 | 1.00 | 10.68 | 7 | 2599 | CB BILE A 325 | 38.139 | 64.627 | 43.330 | 0.40 | 12.90 | 6 |
| 2562 | CA LEU A 321  | 24.610 | 68.918 | 42.896 | 1.00 | 10.60 | 6 | 2600 | CGIBILE A 325 | 37.386 | 64.127 | 44.568 | 0.40 | 10.36 | 6 |
| 2563 | C LEU A 321   | 25.415 | 67.643 | 42.685 | 1.00 | 10.70 | 6 | 2601 | CG2BILE A 325 | 39.604 | 64.862 | 43.640 | 0.40 | 10.82 | 6 |
| 2564 | O LEU A 321   | 25.448 | 66.685 | 43.452 | 1.00 | 11.96 | 8 | 2602 | CDIBILE A 325 | 37.571 | 62.651 | 44.847 | 0.40 | 13.69 | 6 |
| 2565 | CB LEU A 321  | 25.299 | 69.733 | 44.024 | 1.00 | 9.53  | 6 | 2603 | N ASP A 326   | 38.028 | 65.680 | 40.350 | 1.00 | 9.63  | 7 |
| 2566 | CG LEU A 321  | 24.761 | 71.176 | 44.124 | 1.00 | 9.68  | 6 | 2604 | CA ASP A 326  | 38.762 | 65.987 | 39.107 | 1.00 | 10.15 | 6 |
| 2567 | CD1 LEU A 321 | 25.310 | 71.820 | 45.415 | 1.00 | 13.05 | 6 | 2605 | C ASP A 326   | 37.813 | 65.625 | 37.964 | 1.00 | 11.71 | 6 |
| 2568 | CD2 LEU A 321 | 25.183 | 72.064 | 42.930 | 1.00 | 9.85  | 6 | 2606 | O ASP A 326   | 36.678 | 65.102 | 38.209 | 1.00 | 10.86 | 8 |
| 2569 | N ILE A 322   | 26.185 | 67.671 | 41.566 | 1.00 | 9.04  | 7 | 2607 | CB ASP A 326  | 40.149 | 65.323 | 39.050 | 1.00 | 12.00 | 6 |
| 2570 | CA ILE A 322  | 27.014 | 66.478 | 41.265 | 1.00 | 9.68  | 6 | 2608 | CG ASP A 326  | 40.166 | 63.807 | 39.089 | 1.00 | 12.49 | 6 |
| 2571 | C ILE A 322   | 28.477 | 66.821 | 41.584 | 1.00 | 11.13 | 6 | 2609 | OD1 ASP A 326 | 39.080 | 63.207 | 38.870 | 1.00 | 12.13 | 8 |
| 2572 | O ILE A 322   | 29.071 | 67.716 | 40.935 | 1.00 | 10.40 | 8 | 2610 | OD2 ASP A 326 | 41.228 | 63.200 | 39.354 | 1.00 | 11.72 | 8 |
| 2573 | CB ILE A 322  | 26.872 | 66.118 | 39.767 | 1.00 | 10.10 | 6 | 2611 | N ASN A 327   | 38.279 | 65.749 | 36.731 | 1.00 | 9.05  | 7 |
| 2574 | CG1 ILE A 322 | 25.387 | 65.842 | 39.384 | 1.00 | 9.96  | 6 | 2612 | CA ASN A 327  | 37.486 | 65.359 | 35.569 | 1.00 | 10.52 | 6 |
| 2575 | CG2 ILE A 322 | 27.793 | 64.954 | 39.396 | 1.00 | 12.80 | 6 | 2613 | C ASN A 327   | 38.334 | 65.556 | 34.352 | 1.00 | 9.98  | 6 |
| 2576 | CD1 ILE A 322 | 24.773 | 64.698 | 40.258 | 1.00 | 9.05  | 6 | 2614 | O ASN A 327   | 39.573 | 65.686 | 34.478 | 1.00 | 11.19 | 8 |
| 2577 | N THR A 323   | 29.019 | 66.133 | 42.594 | 1.00 | 9.87  | 7 | 2615 | CB ASN A 327  | 36.177 | 66.162 | 35.432 | 1.00 | 11.56 | 6 |
| 2578 | CA THR A 323  | 30.333 | 66.524 | 43.130 | 1.00 | 8.82  | 6 | 2616 | CG ASN A 327  | 36.351 | 67.636 | 35.121 | 1.00 | 12.65 | 6 |
| 2579 | C THR A 323   | 31.433 | 65.704 | 42.453 | 1.00 | 9.73  | 6 | 2617 | OD1 ASN A 327 | 37.355 | 68.106 | 34.634 | 1.00 | 11.48 | 8 |
| 2580 | O THR A 323   | 31.218 | 64.628 | 41.902 | 1.00 | 10.64 | 8 | 2618 | ND2 ASN A 327 | 35.314 | 68.376 | 35.463 | 1.00 | 8.99  | 7 |
| 2581 | CB THR A 323  | 30.364 | 66.302 | 44.652 | 1.00 | 10.77 | 6 | 2619 | N HIS A 328   | 37.802 | 65.385 | 33.178 | 1.00 | 9.23  | 7 |
| 2582 | CG1 THR A 323 | 30.009 | 64.919 | 44.887 | 1.00 | 10.73 | 8 | 2620 | CA HIS A 328  | 38.599 | 65.393 | 31.958 | 1.00 | 11.14 | 6 |
| 2583 | CG2 THR A 323 | 29.314 | 67.237 | 45.318 | 1.00 | 10.06 | 6 | 2621 | C HIS A 328   | 39.037 | 66.779 | 31.471 | 1.00 | 11.62 | 6 |
| 2584 | N PHE A 324   | 32.660 | 66.234 | 42.559 | 1.00 | 9.44  | 7 | 2622 | O HIS A 328   | 39.744 | 66.836 | 30.450 | 1.00 | 11.55 | 8 |
| 2585 | CA PHE A 324  | 33.784 | 65.582 | 41.880 | 1.00 | 10.80 | 6 | 2623 | CB HIS A 328  | 37.726 | 64.740 | 30.844 | 1.00 | 10.61 | 6 |
| 2586 | C PHE A 324   | 35.086 | 66.205 | 42.385 | 1.00 | 9.58  | 6 | 2624 | CG HIS A 328  | 36.511 | 65.577 | 30.526 | 1.00 | 9.76  | 6 |
| 2587 | O PHE A 324   | 35.086 | 67.375 | 42.805 | 1.00 | 10.73 | 8 | 2625 | ND1 HIS A 328 | 35.652 | 65.938 | 31.572 | 1.00 | 11.58 | 7 |
| 2588 | CB PHE A 324  | 33.716 | 65.698 | 40.286 | 1.00 | 9.57  | 6 | 2626 | CD2 HIS A 328 | 36.012 | 66.093 | 29.370 | 1.00 | 11.35 | 6 |
| 2589 | CG PHE A 324  | 33.638 | 67.122 | 39.817 | 1.00 | 9.02  | 6 | 2627 | CE1 HIS A 328 | 34.648 | 66.668 | 31.066 | 1.00 | 12.44 | 6 |
| 2590 | CD1 PHE A 324 | 32.421 | 67.817 | 39.810 | 1.00 | 11.94 | 6 | 2628 | NE2 HIS A 328 | 34.853 | 66.756 | 29.733 | 1.00 | 11.88 | 7 |
| 2591 | CD2 PHE A 324 | 34.798 | 67.746 | 39.354 | 1.00 | 11.07 | 6 | 2629 | N ASP A 329   | 38.746 | 67.808 | 32.263 | 1.00 | 8.48  | 7 |
| 2592 | CE1 PHE A 324 | 32.321 | 69.142 | 39.380 | 1.00 | 11.10 | 6 | 2630 | CA ASP A 329  | 39.181 | 69.155 | 31.893 | 1.00 | 9.03  | 6 |
| 2593 | CE2 PHE A 324 | 34.683 | 69.083 | 38.926 | 1.00 | 11.33 | 6 | 2631 | C ASP A 329   | 40.073 | 69.793 | 32.960 | 1.00 | 12.15 | 6 |
| 2594 | CZ PHE A 324  | 33.498 | 69.788 | 38.931 | 1.00 | 13.68 | 6 | 2632 | O ASP A 329   | 40.388 | 71.012 | 32.883 | 1.00 | 12.94 | 8 |
| 2595 | N ILE A 325   | 36.137 | 65.385 | 42.285 | 1.00 | 9.28  | 7 | 2633 | CB ASP A 329  | 37.955 | 70.091 | 31.837 | 1.00 | 11.03 | 6 |
| 2596 | CA ILE A 325  | 37.469 | 65.879 | 42.710 | 1.00 | 9.24  | 6 | 2634 | CG ASP A 329  | 37.069 | 69.815 | 30.620 | 1.00 | 11.95 | 6 |
| 2597 | C ILE A 325   | 38.277 | 66.277 | 41.480 | 1.00 | 9.67  | 6 | 2635 | OD1 ASP A 329 | 37.477 | 69.188 | 29.617 | 1.00 | 11.39 | 8 |
| 2598 | O ILE A 325   | 39.255 | 67.116 | 41.645 | 1.00 | 10.76 | 8 | 2636 | OD2 ASP A 329 | 35.891 | 70.243 | 30.712 | 1.00 | 11.11 | 8 |
| 2599 | CB AILE A 325 | 38.211 | 64.869 | 43.596 | 0.60 | 11.75 | 6 | 2637 | N MET A 330   | 40.568 | 68.936 | 33.857 | 1.00 | 11.19 | 7 |
| 2600 | CGIAILE A 325 | 38.779 | 63.705 | 42.764 | 0.60 | 10.90 | 6 | 2638 | CA MET A 330  | 41.533 | 69.433 | 34.857 | 1.00 | 9.36  | 6 |





|      |     |           |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2723 | CE  | LVS A 340 | 48.937 | 54.658 | 44.699 | 1.00 | 18.65 | 6 | 2765 | N   | ALA A 346 | 39.590 | 62.418 | 49.883 | 1.00 | 11.81 | 7 |
| 2724 | NZ  | LVS A 340 | 50.377 | 55.099 | 44.564 | 1.00 | 22.63 | 7 | 2766 | CA  | ALA A 346 | 38.762 | 63.250 | 48.987 | 1.00 | 10.44 | 6 |
| 2725 | N   | ALA A 341 | 46.585 | 58.363 | 50.345 | 1.00 | 12.85 | 7 | 2767 | C   | ALA A 346 | 37.604 | 62.379 | 48.462 | 1.00 | 11.17 | 6 |
| 2726 | CA  | ALA A 341 | 45.626 | 58.557 | 51.453 | 1.00 | 14.45 | 6 | 2768 | O   | ALA A 346 | 36.473 | 62.887 | 48.339 | 1.00 | 11.30 | 8 |
| 2727 | C   | ALA A 341 | 44.835 | 59.830 | 51.239 | 1.00 | 13.48 | 6 | 2769 | CB  | ALA A 346 | 39.595 | 63.827 | 47.829 | 1.00 | 9.34  | 6 |
| 2728 | O   | ALA A 341 | 43.661 | 59.855 | 51.568 | 1.00 | 11.31 | 8 | 2770 | N   | LEU A 347 | 37.895 | 61.107 | 48.079 | 1.00 | 12.34 | 7 |
| 2729 | CB  | ALA A 341 | 46.346 | 58.628 | 52.806 | 1.00 | 15.23 | 6 | 2771 | CA  | LEU A 347 | 36.809 | 60.261 | 47.589 | 1.00 | 11.12 | 6 |
| 2730 | N   | ASN A 342 | 45.459 | 60.911 | 50.731 | 1.00 | 10.37 | 7 | 2772 | C   | LEU A 347 | 35.777 | 59.999 | 48.733 | 1.00 | 9.98  | 6 |
| 2731 | CA  | ASN A 342 | 44.717 | 62.126 | 50.470 | 1.00 | 10.38 | 6 | 2773 | O   | LEU A 347 | 34.567 | 60.087 | 48.466 | 1.00 | 11.63 | 8 |
| 2732 | C   | ASN A 342 | 43.687 | 61.897 | 49.359 | 1.00 | 10.62 | 6 | 2774 | CB  | LEU A 347 | 37.367 | 58.885 | 47.187 | 1.00 | 11.26 | 6 |
| 2733 | O   | ASN A 342 | 42.560 | 62.477 | 49.439 | 1.00 | 12.01 | 8 | 2775 | CG  | LEU A 347 | 38.146 | 58.913 | 45.840 | 1.00 | 14.75 | 6 |
| 2734 | CB  | ASN A 342 | 45.708 | 63.276 | 50.141 | 1.00 | 11.46 | 6 | 2776 | CD1 | LEU A 347 | 38.829 | 57.574 | 45.530 | 1.00 | 13.09 | 6 |
| 2735 | CG  | ASN A 342 | 46.519 | 63.737 | 51.351 | 1.00 | 13.17 | 6 | 2777 | CD2 | LEU A 347 | 37.132 | 59.197 | 44.722 | 1.00 | 15.41 | 6 |
| 2736 | OD1 | ASN A 342 | 47.710 | 64.044 | 51.127 | 1.00 | 12.82 | 8 | 2778 | N   | ALA A 348 | 36.304 | 59.764 | 49.955 | 1.00 | 10.14 | 7 |
| 2737 | ND2 | ASN A 342 | 45.888 | 63.859 | 52.516 | 1.00 | 12.05 | 7 | 2779 | CA  | ALA A 348 | 35.269 | 59.479 | 51.003 | 1.00 | 10.67 | 6 |
| 2738 | N   | LEU A 343 | 44.001 | 61.049 | 48.344 | 1.00 | 10.66 | 7 | 2780 | C   | ALA A 348 | 34.432 | 60.725 | 51.273 | 1.00 | 12.22 | 6 |
| 2739 | CA  | LEU A 343 | 42.953 | 60.715 | 47.377 | 1.00 | 10.18 | 6 | 2781 | O   | ALA A 348 | 33.231 | 60.600 | 51.534 | 1.00 | 11.88 | 8 |
| 2740 | C   | LEU A 343 | 41.810 | 59.935 | 48.039 | 1.00 | 12.28 | 6 | 2782 | CB  | ALA A 348 | 36.008 | 59.130 | 52.310 | 1.00 | 10.16 | 6 |
| 2741 | O   | LEU A 343 | 40.635 | 60.288 | 47.781 | 1.00 | 11.44 | 8 | 2783 | N   | PHE A 349 | 35.026 | 61.922 | 51.160 | 1.00 | 10.08 | 7 |
| 2742 | CB  | LEU A 343 | 43.581 | 59.854 | 46.229 | 1.00 | 10.02 | 6 | 2784 | CA  | PHE A 349 | 34.258 | 63.149 | 51.330 | 1.00 | 10.26 | 6 |
| 2743 | CG  | LEU A 343 | 42.546 | 59.182 | 45.295 | 1.00 | 10.27 | 6 | 2785 | C   | PHE A 349 | 33.120 | 63.213 | 50.282 | 1.00 | 9.67  | 6 |
| 2744 | CD1 | LEU A 343 | 41.847 | 60.288 | 44.550 | 1.00 | 13.59 | 6 | 2786 | O   | PHE A 349 | 31.942 | 63.422 | 50.717 | 1.00 | 11.25 | 8 |
| 2745 | CD2 | LEU A 343 | 43.309 | 58.294 | 44.283 | 1.00 | 12.64 | 6 | 2787 | CB  | PHE A 349 | 35.270 | 64.348 | 51.200 | 1.00 | 9.92  | 6 |
| 2746 | N   | HIS A 344 | 42.173 | 58.977 | 48.898 | 1.00 | 11.47 | 7 | 2788 | CG  | PHE A 349 | 34.515 | 65.659 | 51.357 | 1.00 | 8.60  | 6 |
| 2747 | CA  | HIS A 344 | 41.093 | 58.185 | 49.570 | 1.00 | 11.49 | 6 | 2789 | CD1 | PHE A 349 | 34.016 | 66.030 | 52.605 | 1.00 | 11.80 | 6 |
| 2748 | C   | HIS A 344 | 40.189 | 59.122 | 50.370 | 1.00 | 13.40 | 6 | 2790 | CD2 | PHE A 349 | 34.340 | 66.526 | 50.249 | 1.00 | 11.51 | 6 |
| 2749 | O   | HIS A 344 | 38.951 | 58.916 | 50.500 | 1.00 | 12.11 | 8 | 2791 | CE1 | PHE A 349 | 33.296 | 67.247 | 52.714 | 1.00 | 11.90 | 6 |
| 2750 | CB  | HIS A 344 | 41.731 | 57.075 | 50.439 | 1.00 | 9.09  | 6 | 2792 | CE2 | PHE A 349 | 33.638 | 67.709 | 50.409 | 1.00 | 10.49 | 6 |
| 2751 | CG  | HIS A 344 | 42.520 | 56.064 | 49.656 | 1.00 | 10.04 | 6 | 2793 | CZ  | PHE A 349 | 33.069 | 68.068 | 51.660 | 1.00 | 12.88 | 6 |
| 2752 | ND1 | HIS A 344 | 43.612 | 55.436 | 50.199 | 1.00 | 12.75 | 7 | 2794 | N   | ILE A 350 | 33.411 | 63.030 | 49.005 | 1.00 | 8.49  | 7 |
| 2753 | CD2 | HIS A 344 | 42.363 | 55.580 | 48.370 | 1.00 | 11.63 | 6 | 2795 | CA  | ILE A 350 | 32.257 | 63.124 | 48.089 | 1.00 | 10.97 | 6 |
| 2754 | CE1 | HIS A 344 | 44.114 | 54.612 | 49.289 | 1.00 | 10.72 | 6 | 2796 | C   | ILE A 350 | 31.361 | 61.899 | 48.158 | 1.00 | 11.48 | 6 |
| 2755 | NE2 | HIS A 344 | 43.393 | 54.662 | 48.157 | 1.00 | 12.61 | 7 | 2797 | O   | ILE A 350 | 30.139 | 62.115 | 47.958 | 1.00 | 11.30 | 8 |
| 2756 | N   | GLN A 345 | 40.834 | 60.100 | 51.024 | 1.00 | 10.53 | 7 | 2798 | CB  | ILE A 350 | 32.676 | 63.380 | 46.605 | 1.00 | 11.26 | 6 |
| 2757 | CA  | GLN A 345 | 40.049 | 61.036 | 51.831 | 1.00 | 10.43 | 6 | 2799 | CG1 | ILE A 350 | 33.451 | 62.279 | 45.983 | 1.00 | 11.16 | 6 |
| 2758 | C   | GLN A 345 | 39.077 | 61.899 | 51.008 | 1.00 | 10.42 | 6 | 2800 | CG2 | ILE A 350 | 33.429 | 64.742 | 46.556 | 1.00 | 12.07 | 6 |
| 2759 | O   | GLN A 345 | 37.888 | 62.067 | 51.324 | 1.00 | 10.38 | 8 | 2801 | CD1 | ILE A 350 | 33.748 | 62.454 | 44.463 | 1.00 | 9.59  | 6 |
| 2760 | CB  | GLN A 345 | 40.996 | 62.012 | 52.564 | 1.00 | 11.01 | 6 | 2802 | N   | LEU A 351 | 31.873 | 60.731 | 48.548 | 1.00 | 9.78  | 7 |
| 2761 | CG  | GLN A 345 | 41.847 | 61.258 | 53.641 | 1.00 | 9.73  | 6 | 2803 | CA  | LEU A 351 | 30.930 | 59.601 | 48.655 | 1.00 | 9.90  | 6 |
| 2762 | CD  | GLN A 345 | 43.142 | 62.041 | 53.786 | 1.00 | 10.78 | 6 | 2804 | C   | LEU A 351 | 29.956 | 59.782 | 49.809 | 1.00 | 11.10 | 6 |
| 2763 | OE1 | GLN A 345 | 43.232 | 63.196 | 53.279 | 1.00 | 12.69 | 8 | 2805 | O   | LEU A 351 | 28.888 | 59.122 | 49.698 | 1.00 | 11.60 | 6 |
| 2764 | NE2 | GLN A 345 | 44.170 | 61.448 | 54.428 | 1.00 | 12.87 | 7 | 2806 | CB  | LEU A 351 | 31.813 | 58.349 | 48.879 | 1.00 | 11.35 | 6 |







|      |               |        |        |        |      |       |   |      |               |        |        |        |      |       |   |
|------|---------------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 3055 | OD1 ASP A 383 | 43.286 | 44.428 | 41.805 | 1.00 | 20.99 | 8 | 3097 | CD2 PHE A 389 | 37.375 | 48.299 | 41.777 | 1.00 | 14.39 | 6 |
| 3056 | OD2 ASP A 383 | 45.229 | 45.408 | 41.363 | 1.00 | 21.43 | 8 | 3098 | CE1 PHE A 389 | 35.869 | 46.515 | 43.383 | 1.00 | 14.50 | 6 |
| 3057 | N THR A 384   | 40.302 | 44.680 | 40.950 | 1.00 | 13.75 | 7 | 3099 | CE2 PHE A 389 | 36.340 | 47.536 | 41.216 | 1.00 | 12.44 | 6 |
| 3058 | CA THR A 384  | 39.215 | 44.894 | 41.930 | 1.00 | 12.49 | 6 | 3100 | CZ PHE A 389  | 35.646 | 46.648 | 42.031 | 1.00 | 13.69 | 6 |
| 3059 | C THR A 384   | 39.773 | 44.871 | 43.345 | 1.00 | 13.78 | 6 | 3101 | N LYS A 390   | 38.053 | 49.160 | 46.775 | 1.00 | 12.03 | 7 |
| 3060 | O THR A 384   | 38.951 | 44.852 | 44.298 | 1.00 | 18.13 | 8 | 3102 | CA LYS A 390  | 37.303 | 48.672 | 47.936 | 1.00 | 12.63 | 6 |
| 3061 | CB THR A 384  | 38.098 | 43.831 | 41.755 | 1.00 | 16.42 | 6 | 3103 | C LYS A 390   | 36.544 | 49.767 | 48.699 | 1.00 | 14.75 | 6 |
| 3062 | OG1 THR A 384 | 38.725 | 42.525 | 41.937 | 1.00 | 18.75 | 8 | 3104 | O LYS A 390   | 35.438 | 49.556 | 49.197 | 1.00 | 12.66 | 8 |
| 3063 | CG2 THR A 384 | 37.515 | 43.943 | 40.342 | 1.00 | 20.28 | 6 | 3105 | CB LYS A 390  | 38.291 | 48.000 | 48.917 | 1.00 | 12.06 | 6 |
| 3064 | N THR A 385   | 41.088 | 44.832 | 43.573 | 1.00 | 14.37 | 7 | 3106 | CG LYS A 390  | 38.798 | 46.712 | 48.243 | 1.00 | 15.90 | 6 |
| 3065 | CA THR A 385  | 41.648 | 44.691 | 44.906 | 1.00 | 16.71 | 6 | 3107 | CD LYS A 390  | 39.589 | 45.970 | 49.325 | 1.00 | 25.81 | 6 |
| 3066 | C THR A 385   | 42.313 | 45.974 | 45.424 | 1.00 | 16.63 | 6 | 3108 | CE LYS A 390  | 40.980 | 46.524 | 49.440 | 1.00 | 29.79 | 6 |
| 3067 | O THR A 385   | 42.873 | 45.952 | 46.539 | 1.00 | 14.22 | 8 | 3109 | NZ LYS A 390  | 41.835 | 45.465 | 50.107 | 1.00 | 41.01 | 7 |
| 3068 | CB THR A 385  | 42.693 | 43.546 | 45.009 | 1.00 | 19.15 | 6 | 3110 | N GLU A 391   | 37.256 | 50.908 | 48.782 | 1.00 | 11.21 | 7 |
| 3069 | OG1 THR A 385 | 43.883 | 43.878 | 44.288 | 1.00 | 17.99 | 8 | 3111 | CA GLU A 391  | 36.636 | 52.048 | 49.475 | 1.00 | 11.43 | 6 |
| 3070 | CG2 THR A 385 | 42.075 | 42.234 | 44.541 | 1.00 | 24.33 | 6 | 3112 | C GLU A 391   | 35.375 | 52.482 | 48.742 | 1.00 | 12.51 | 6 |
| 3071 | N THR A 386   | 42.254 | 47.039 | 44.606 | 1.00 | 14.92 | 7 | 3113 | O GLU A 391   | 34.300 | 52.735 | 49.337 | 1.00 | 10.64 | 8 |
| 3072 | CA THR A 386  | 42.952 | 48.254 | 45.131 | 1.00 | 13.63 | 6 | 3114 | CB GLU A 391  | 37.670 | 53.223 | 49.487 | 1.00 | 10.44 | 6 |
| 3073 | C THR A 386   | 42.175 | 48.801 | 46.328 | 1.00 | 11.22 | 6 | 3115 | CG GLU A 391  | 36.957 | 54.519 | 49.997 | 1.00 | 10.67 | 6 |
| 3074 | O THR A 386   | 40.990 | 48.649 | 46.478 | 1.00 | 12.74 | 8 | 3116 | CD GLU A 391  | 37.870 | 55.744 | 49.810 | 1.00 | 12.38 | 6 |
| 3075 | CB THR A 386  | 43.101 | 49.344 | 44.054 | 1.00 | 13.50 | 6 | 3117 | OE1 GLU A 391 | 38.974 | 55.628 | 49.226 | 1.00 | 13.12 | 8 |
| 3076 | OG1 THR A 386 | 41.805 | 49.919 | 43.822 | 1.00 | 12.14 | 8 | 3118 | OE2 GLU A 391 | 37.458 | 56.841 | 50.284 | 1.00 | 12.94 | 8 |
| 3077 | CG2 THR A 386 | 43.656 | 48.809 | 42.719 | 1.00 | 17.62 | 6 | 3119 | N VAL A 392   | 35.455 | 52.675 | 47.403 | 1.00 | 11.36 | 7 |
| 3078 | N THR A 387   | 42.886 | 49.552 | 47.184 | 1.00 | 14.21 | 7 | 3120 | CA VAL A 392  | 34.279 | 53.176 | 46.653 | 1.00 | 12.25 | 6 |
| 3079 | CA THR A 387  | 42.237 | 50.167 | 48.316 | 1.00 | 11.44 | 6 | 3121 | C VAL A 392   | 33.156 | 52.128 | 46.716 | 1.00 | 12.76 | 6 |
| 3080 | C THR A 387   | 41.127 | 51.134 | 47.887 | 1.00 | 12.54 | 6 | 3122 | CB VAL A 392  | 31.968 | 52.481 | 46.930 | 1.00 | 12.77 | 8 |
| 3081 | O THR A 387   | 40.045 | 51.113 | 48.437 | 1.00 | 12.57 | 8 | 3123 | CB VAL A 392  | 34.667 | 53.410 | 45.175 | 1.00 | 14.39 | 6 |
| 3082 | CB THR A 387  | 43.277 | 50.926 | 49.145 | 1.00 | 17.16 | 6 | 3124 | CG1 VAL A 392 | 33.434 | 53.661 | 44.296 | 1.00 | 13.75 | 6 |
| 3083 | OG1 THR A 387 | 44.177 | 49.939 | 49.669 | 1.00 | 15.42 | 8 | 3125 | CG2 VAL A 392 | 35.702 | 54.570 | 45.061 | 1.00 | 12.07 | 6 |
| 3084 | CG2 THR A 387 | 42.644 | 51.724 | 50.273 | 1.00 | 14.27 | 6 | 3126 | N SER A 393   | 33.487 | 50.846 | 46.628 | 1.00 | 10.90 | 7 |
| 3085 | N ALA A 388   | 41.441 | 51.910 | 46.838 | 1.00 | 13.30 | 7 | 3127 | CA SER A 393  | 32.426 | 49.822 | 46.686 | 1.00 | 12.19 | 6 |
| 3086 | CA ALA A 388  | 40.376 | 52.785 | 46.360 | 1.00 | 10.83 | 6 | 3128 | C SER A 393   | 31.708 | 49.782 | 48.021 | 1.00 | 10.96 | 6 |
| 3087 | C ALA A 388   | 39.162 | 52.083 | 45.808 | 1.00 | 12.23 | 6 | 3129 | O SER A 393   | 30.469 | 49.774 | 48.186 | 1.00 | 12.48 | 8 |
| 3088 | O ALA A 388   | 38.030 | 52.497 | 46.001 | 1.00 | 11.44 | 8 | 3130 | CB SER A 393  | 33.059 | 48.431 | 46.394 | 1.00 | 12.79 | 6 |
| 3089 | CB ALA A 388  | 40.968 | 53.700 | 45.239 | 1.00 | 10.26 | 6 | 3131 | OG SER A 393  | 31.944 | 47.538 | 46.423 | 1.00 | 19.93 | 8 |
| 3090 | N PHE A 389   | 39.347 | 50.956 | 45.084 | 1.00 | 12.53 | 7 | 3132 | N THR A 394   | 32.493 | 49.942 | 49.099 | 1.00 | 11.04 | 7 |
| 3091 | CA PHE A 389  | 38.202 | 50.182 | 44.579 | 1.00 | 13.64 | 6 | 3133 | CA THR A 394  | 31.920 | 49.922 | 50.445 | 1.00 | 12.34 | 6 |
| 3092 | C PHE A 389   | 37.361 | 49.746 | 45.779 | 1.00 | 13.47 | 6 | 3134 | C THR A 394   | 31.061 | 51.130 | 50.682 | 1.00 | 11.80 | 6 |
| 3093 | O PHE A 389   | 36.157 | 49.895 | 45.789 | 1.00 | 12.37 | 8 | 3135 | O THR A 394   | 29.935 | 51.097 | 51.169 | 1.00 | 11.63 | 8 |
| 3094 | CB PHE A 389  | 38.766 | 48.975 | 43.763 | 1.00 | 11.46 | 6 | 3136 | CB THR A 394  | 33.039 | 49.889 | 51.509 | 1.00 | 12.40 | 6 |
| 3095 | CG PHE A 389  | 37.627 | 48.178 | 43.141 | 1.00 | 12.01 | 6 | 3137 | OG1 THR A 394 | 33.699 | 48.614 | 51.401 | 1.00 | 14.67 | 8 |
| 3096 | CD1 PHE A 389 | 36.936 | 47.248 | 43.916 | 1.00 | 16.87 | 6 | 3138 | CG2 THR A 394 | 32.443 | 50.011 | 52.927 | 1.00 | 14.84 | 6 |









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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3391 | N   | LVS A 425 | 22.068 | 63.623 | 58.542 | 1.00 | 11.90 | 7 | 3433 | O   | ASP A 429 | 20.026 | 60.024 | 59.967 | 1.00 | 13.16 | 8 |
| 3392 | CA  | LVS A 425 | 20.937 | 63.080 | 59.290 | 1.00 | 11.75 | 6 | 3434 | CB  | ASP A 429 | 18.927 | 57.501 | 58.471 | 1.00 | 12.81 | 6 |
| 3393 | C   | LVS A 425 | 19.685 | 63.233 | 58.443 | 1.00 | 15.39 | 6 | 3435 | CG  | ASP A 429 | 17.766 | 56.561 | 58.255 | 1.00 | 28.25 | 6 |
| 3394 | O   | LVS A 425 | 19.444 | 64.340 | 58.036 | 1.00 | 14.23 | 8 | 3436 | OD1 | ASP A 429 | 17.727 | 55.530 | 58.940 | 1.00 | 20.84 | 8 |
| 3395 | CB  | LVS A 425 | 20.801 | 63.854 | 60.626 | 1.00 | 13.68 | 6 | 3437 | OD2 | ASP A 429 | 16.804 | 56.870 | 57.490 | 1.00 | 27.47 | 8 |
| 3396 | CG  | LVS A 425 | 19.617 | 63.271 | 61.494 | 1.00 | 14.44 | 6 | 3438 | N   | VAL A 430 | 21.384 | 58.297 | 60.600 | 1.00 | 12.85 | 7 |
| 3397 | CD  | LVS A 425 | 19.721 | 63.992 | 62.863 | 1.00 | 19.53 | 6 | 3439 | CA  | VAL A 430 | 22.502 | 59.192 | 60.876 | 1.00 | 11.51 | 6 |
| 3398 | CE  | LVS A 425 | 18.739 | 63.342 | 63.856 | 1.00 | 20.97 | 6 | 3440 | C   | VAL A 430 | 23.816 | 58.621 | 60.371 | 1.00 | 13.31 | 6 |
| 3399 | NZ  | LVS A 425 | 17.322 | 63.663 | 63.509 | 1.00 | 23.72 | 7 | 3441 | O   | VAL A 430 | 23.993 | 57.405 | 60.522 | 1.00 | 12.49 | 8 |
| 3400 | N   | PHE A 426 | 18.908 | 62.144 | 58.357 | 1.00 | 12.33 | 7 | 3442 | CB  | VAL A 430 | 22.632 | 59.315 | 62.427 | 1.00 | 14.21 | 6 |
| 3401 | CA  | PHE A 426 | 17.583 | 62.238 | 57.709 | 1.00 | 12.03 | 6 | 3443 | CG1 | VAL A 430 | 23.828 | 60.233 | 62.734 | 1.00 | 14.56 | 6 |
| 3402 | C   | PHE A 426 | 16.651 | 61.481 | 58.706 | 1.00 | 11.05 | 6 | 3444 | CG2 | VAL A 430 | 21.373 | 59.955 | 63.033 | 1.00 | 14.79 | 6 |
| 3403 | O   | PHE A 426 | 16.657 | 60.252 | 58.693 | 1.00 | 13.03 | 8 | 3445 | N   | VAL A 431 | 24.721 | 59.432 | 59.826 | 1.00 | 12.54 | 7 |
| 3404 | CB  | PHE A 426 | 17.608 | 61.450 | 56.397 | 1.00 | 13.23 | 6 | 3446 | CA  | VAL A 431 | 26.043 | 58.933 | 59.434 | 1.00 | 11.58 | 6 |
| 3405 | CG  | PHE A 426 | 16.260 | 61.449 | 55.699 | 1.00 | 12.58 | 6 | 3447 | C   | VAL A 431 | 27.051 | 59.978 | 59.912 | 1.00 | 11.43 | 6 |
| 3406 | CD1 | PHE A 426 | 15.838 | 62.659 | 55.147 | 1.00 | 14.04 | 6 | 3448 | O   | VAL A 431 | 26.847 | 61.129 | 59.603 | 1.00 | 12.12 | 8 |
| 3407 | CD2 | PHE A 426 | 15.515 | 60.300 | 55.571 | 1.00 | 14.55 | 6 | 3449 | CB  | VAL A 431 | 26.250 | 58.685 | 57.905 | 1.00 | 12.54 | 6 |
| 3408 | CE1 | PHE A 426 | 14.594 | 62.715 | 54.490 | 1.00 | 13.58 | 6 | 3450 | CG1 | VAL A 431 | 27.698 | 58.199 | 57.615 | 1.00 | 10.81 | 6 |
| 3409 | CE2 | PHE A 426 | 14.264 | 60.345 | 54.906 | 1.00 | 15.67 | 6 | 3451 | CG2 | VAL A 431 | 25.254 | 57.657 | 57.400 | 1.00 | 13.14 | 6 |
| 3410 | CZ  | PHE A 426 | 13.839 | 61.552 | 54.398 | 1.00 | 15.62 | 6 | 3452 | N   | LEU A 432 | 27.976 | 59.557 | 60.800 | 1.00 | 10.48 | 7 |
| 3411 | N   | PHE A 427 | 15.916 | 62.357 | 59.408 | 1.00 | 14.34 | 7 | 3453 | CA  | LEU A 432 | 29.015 | 60.512 | 61.285 | 1.00 | 11.27 | 6 |
| 3412 | CA  | PHE A 427 | 15.024 | 61.773 | 60.490 | 1.00 | 16.20 | 6 | 3454 | C   | LEU A 432 | 30.317 | 60.140 | 60.583 | 1.00 | 11.12 | 6 |
| 3413 | C   | PHE A 427 | 15.781 | 60.836 | 61.400 | 1.00 | 17.32 | 6 | 3455 | O   | LEU A 432 | 30.708 | 58.961 | 60.577 | 1.00 | 13.28 | 8 |
| 3414 | O   | PHE A 427 | 16.737 | 61.354 | 62.070 | 1.00 | 19.10 | 8 | 3456 | CB  | LEU A 432 | 29.087 | 60.224 | 62.831 | 1.00 | 11.86 | 6 |
| 3415 | CB  | PHE A 427 | 13.772 | 61.132 | 59.840 | 1.00 | 18.52 | 6 | 3457 | CG  | LEU A 432 | 30.033 | 61.205 | 63.562 | 1.00 | 11.74 | 6 |
| 3416 | CG  | PHE A 427 | 12.888 | 62.175 | 59.193 | 1.00 | 17.73 | 6 | 3458 | CD1 | LEU A 432 | 29.574 | 62.643 | 63.510 | 1.00 | 11.18 | 6 |
| 3417 | CD1 | PHE A 427 | 11.972 | 62.918 | 59.905 | 1.00 | 21.55 | 6 | 3459 | CD2 | LEU A 432 | 30.119 | 60.744 | 65.044 | 1.00 | 14.23 | 6 |
| 3418 | CD2 | PHE A 427 | 13.018 | 62.396 | 57.830 | 1.00 | 14.51 | 6 | 3460 | N   | VAL A 433 | 30.987 | 61.141 | 59.978 | 1.00 | 11.73 | 7 |
| 3419 | CE1 | PHE A 427 | 11.188 | 63.858 | 59.276 | 1.00 | 18.85 | 6 | 3461 | CA  | VAL A 433 | 32.162 | 60.867 | 59.131 | 1.00 | 9.07  | 6 |
| 3420 | CE2 | PHE A 427 | 12.246 | 63.336 | 57.185 | 1.00 | 16.68 | 6 | 3462 | C   | VAL A 433 | 33.328 | 61.667 | 59.702 | 1.00 | 9.49  | 6 |
| 3421 | CZ  | PHE A 427 | 11.311 | 64.087 | 57.906 | 1.00 | 19.85 | 6 | 3463 | O   | VAL A 433 | 33.158 | 62.864 | 59.844 | 1.00 | 10.58 | 8 |
| 3422 | N   | ASN A 428 | 15.546 | 59.522 | 61.442 | 1.00 | 15.71 | 7 | 3464 | CB  | VAL A 433 | 31.899 | 61.334 | 57.674 | 1.00 | 10.62 | 6 |
| 3423 | CA  | ASN A 428 | 16.284 | 58.735 | 62.433 | 1.00 | 17.74 | 6 | 3465 | CG1 | VAL A 433 | 33.173 | 61.088 | 56.812 | 1.00 | 11.05 | 6 |
| 3424 | C   | ASN A 428 | 17.573 | 58.173 | 61.837 | 1.00 | 17.74 | 6 | 3466 | CG2 | VAL A 433 | 30.693 | 60.564 | 57.072 | 1.00 | 11.15 | 6 |
| 3425 | O   | ASN A 428 | 18.307 | 57.587 | 62.639 | 1.00 | 17.57 | 8 | 3467 | N   | ALA A 434 | 34.455 | 61.000 | 60.017 | 1.00 | 10.65 | 7 |
| 3426 | CB  | ASN A 428 | 15.484 | 57.591 | 63.008 | 1.00 | 22.35 | 6 | 3468 | CA  | ALA A 434 | 35.643 | 61.757 | 60.409 | 1.00 | 10.07 | 6 |
| 3427 | CG  | ASN A 428 | 14.267 | 58.214 | 63.733 | 1.00 | 36.36 | 6 | 3469 | C   | ALA A 434 | 36.742 | 61.603 | 59.363 | 1.00 | 11.73 | 6 |
| 3428 | OD1 | ASN A 428 | 14.452 | 59.092 | 64.570 | 1.00 | 38.45 | 8 | 3470 | O   | ALA A 434 | 37.030 | 60.489 | 58.924 | 1.00 | 11.96 | 8 |
| 3429 | ND2 | ASN A 428 | 13.103 | 57.735 | 63.325 | 1.00 | 44.64 | 7 | 3471 | CB  | ALA A 434 | 36.199 | 61.171 | 61.742 | 1.00 | 10.24 | 6 |
| 3430 | N   | ASP A 429 | 17.867 | 58.370 | 60.547 | 1.00 | 15.06 | 7 | 3472 | N   | ILE A 435 | 37.345 | 62.744 | 58.992 | 1.00 | 10.23 | 7 |
| 3431 | CA  | ASP A 429 | 19.091 | 57.810 | 59.986 | 1.00 | 14.19 | 6 | 3473 | CA  | ILE A 435 | 38.438 | 62.741 | 58.008 | 1.00 | 8.82  | 6 |
| 3432 | C   | ASP A 429 | 20.222 | 58.816 | 60.103 | 1.00 | 11.55 | 6 | 3474 | C   | ILE A 435 | 39.571 | 63.587 | 58.558 | 1.00 | 10.58 | 6 |



|      |     |            |        |        |        |            |   |      |     |           |        |        |        |            |   |
|------|-----|------------|--------|--------|--------|------------|---|------|-----|-----------|--------|--------|--------|------------|---|
| 3559 | CG2 | ILE A 445  | 37.159 | 63.906 | 68.223 | 1.00 16.44 | 6 | 3596 | CA  | ALA A 451 | 22.898 | 62.330 | 66.941 | 1.00 16.96 | 6 |
| 3560 | CD1 | ILE A 445  | 39.772 | 64.500 | 66.533 | 1.00 15.53 | 6 | 3597 | C   | ALA A 451 | 22.799 | 60.830 | 66.879 | 1.00 15.04 | 6 |
| 3561 | N   | SER A 446  | 38.309 | 64.925 | 71.580 | 1.00 15.73 | 7 | 3598 | O   | ALA A 451 | 21.681 | 60.282 | 66.900 | 1.00 15.44 | 8 |
| 3562 | CA  | SER A 446  | 37.450 | 65.018 | 72.601 | 1.00 16.64 | 6 | 3599 | CB  | ALA A 451 | 22.212 | 62.946 | 65.681 | 1.00 16.26 | 6 |
| 3563 | C   | SER A 446  | 36.394 | 66.091 | 72.415 | 1.00 18.39 | 6 | 3600 | N   | LEU A 452 | 23.929 | 60.083 | 66.788 | 1.00 14.57 | 7 |
| 3564 | O   | SER A 446  | 36.592 | 67.021 | 71.653 | 1.00 18.43 | 8 | 3601 | CA  | LEU A 452 | 23.803 | 58.623 | 66.814 | 1.00 12.45 | 6 |
| 3565 | CB  | SER A 446  | 38.248 | 65.398 | 73.972 | 1.00 18.77 | 6 | 3602 | C   | LEU A 452 | 23.170 | 58.200 | 68.158 | 1.00 17.32 | 6 |
| 3566 | OG  | SER A 446  | 38.784 | 66.689 | 73.750 | 1.00 24.38 | 8 | 3603 | O   | LEU A 452 | 23.505 | 58.727 | 69.218 | 1.00 17.00 | 8 |
| 3567 | N   | GLY A 447  | 35.263 | 65.958 | 73.091 | 1.00 19.05 | 7 | 3604 | CB  | LEU A 452 | 25.201 | 57.989 | 66.779 | 1.00 14.27 | 6 |
| 3568 | CA  | GLY A 447  | 34.169 | 66.916 | 73.050 | 1.00 17.05 | 6 | 3605 | CG  | LEU A 452 | 25.854 | 58.082 | 65.380 | 1.00 14.43 | 6 |
| 3569 | C   | GLY A 447  | 33.253 | 66.660 | 71.829 | 1.00 20.26 | 6 | 3606 | CD1 | LEU A 452 | 27.344 | 57.716 | 65.610 | 1.00 13.81 | 6 |
| 3570 | O   | GLY A 447  | 32.491 | 67.554 | 71.467 | 1.00 19.38 | 8 | 3607 | CD2 | LEU A 452 | 25.263 | 57.102 | 64.375 | 1.00 14.40 | 6 |
| 3571 | N   | LEU A 448  | 33.487 | 65.502 | 71.171 | 1.00 13.94 | 7 | 3608 | N   | PRO A 453 | 22.383 | 57.163 | 68.080 | 1.00 16.12 | 7 |
| 3572 | CA  | LEU A 448  | 32.625 | 65.262 | 69.967 | 1.00 15.40 | 6 | 3609 | CA  | PRO A 453 | 21.808 | 56.539 | 69.305 | 1.00 18.87 | 6 |
| 3573 | C   | LEU A 448  | 31.245 | 64.853 | 70.386 | 1.00 16.78 | 6 | 3610 | C   | PRO A 453 | 22.936 | 55.882 | 70.090 | 1.00 19.68 | 6 |
| 3574 | O   | LEU A 448  | 31.018 | 63.906 | 71.155 | 1.00 17.47 | 8 | 3611 | O   | PRO A 453 | 24.039 | 55.532 | 69.686 | 1.00 18.19 | 8 |
| 3575 | CB  | LEU A 448  | 33.312 | 64.155 | 69.144 | 1.00 14.08 | 6 | 3612 | CB  | PRO A 453 | 20.796 | 55.523 | 68.880 | 1.00 20.41 | 6 |
| 3576 | CG  | LEU A 448  | 32.578 | 63.628 | 67.903 | 1.00 15.34 | 6 | 3613 | CG  | PRO A 453 | 20.615 | 55.743 | 67.392 | 1.00 21.35 | 6 |
| 3577 | CD1 | LEU A 448  | 32.403 | 64.740 | 66.845 | 1.00 16.18 | 6 | 3614 | CD  | PRO A 453 | 21.806 | 56.582 | 66.872 | 1.00 16.78 | 6 |
| 3578 | CD2 | LEU A 448  | 33.283 | 62.449 | 67.256 | 1.00 13.42 | 6 | 3615 | N   | ASN A 454 | 22.619 | 55.684 | 71.406 | 1.00 14.58 | 7 |
| 3579 | N   | GLN A 449  | 30.221 | 65.509 | 69.814 | 1.00 13.16 | 7 | 3616 | CA  | ASN A 454 | 23.630 | 55.025 | 72.244 | 1.00 14.89 | 6 |
| 3580 | CA  | GLN A 449  | 28.812 | 65.224 | 70.018 | 1.00 14.91 | 6 | 3617 | C   | ASN A 454 | 24.085 | 53.704 | 71.712 | 1.00 18.47 | 6 |
| 3581 | C   | GLN A 449  | 28.209 | 64.630 | 68.734 | 1.00 16.76 | 6 | 3618 | O   | ASN A 454 | 23.320 | 52.881 | 71.168 | 1.00 17.84 | 8 |
| 3582 | O   | GLN A 449  | 28.754 | 64.827 | 67.645 | 1.00 13.94 | 8 | 3619 | CB  | ASN A 454 | 22.851 | 54.705 | 73.573 | 1.00 17.80 | 6 |
| 3583 | CB  | AGLN A 449 | 28.054 | 66.486 | 70.470 | 0.50 18.23 | 6 | 3620 | CG  | ASN A 454 | 22.656 | 55.933 | 74.421 | 1.00 24.08 | 8 |
| 3584 | CG  | AGLN A 449 | 28.884 | 67.206 | 71.540 | 0.50 24.01 | 6 | 3621 | OD1 | ASN A 454 | 23.071 | 57.055 | 74.201 | 1.00 19.24 | 6 |
| 3585 | CD  | AGLN A 449 | 28.211 | 68.188 | 72.449 | 0.50 23.44 | 6 | 3622 | ND2 | ASN A 454 | 21.941 | 55.757 | 75.554 | 1.00 24.42 | 7 |
| 3586 | OE1 | AGLN A 449 | 28.812 | 68.606 | 73.455 | 0.50 32.55 | 8 | 3623 | N   | GLY A 455 | 25.378 | 53.451 | 71.950 | 1.00 17.75 | 7 |
| 3587 | NE2 | AGLN A 449 | 26.984 | 68.573 | 72.134 | 0.50 32.22 | 7 | 3624 | CA  | GLY A 455 | 25.919 | 52.156 | 71.553 | 1.00 20.13 | 6 |
| 3588 | CB  | BGLN A 449 | 27.974 | 66.473 | 70.339 | 0.50 13.26 | 6 | 3625 | C   | GLY A 455 | 27.422 | 52.289 | 71.172 | 1.00 17.39 | 6 |
| 3589 | CG  | BGLN A 449 | 28.536 | 67.122 | 71.620 | 0.50 17.72 | 6 | 3626 | O   | GLY A 455 | 27.899 | 53.393 | 71.080 | 1.00 19.07 | 8 |
| 3590 | CD  | BGLN A 449 | 28.037 | 66.396 | 72.844 | 0.50 16.00 | 6 | 3627 | N   | SER A 456 | 27.916 | 51.112 | 70.814 | 1.00 18.37 | 7 |
| 3591 | OE1 | BGLN A 449 | 28.776 | 65.702 | 73.511 | 0.50 22.43 | 8 | 3628 | CA  | SER A 456 | 29.286 | 51.073 | 70.261 | 1.00 17.34 | 6 |
| 3592 | NE2 | BGLN A 449 | 26.759 | 66.550 | 73.145 | 0.50 23.34 | 7 | 3629 | C   | SER A 456 | 29.173 | 50.927 | 68.725 | 1.00 17.80 | 6 |
| 3593 | N   | THR A 450  | 27.085 | 63.965 | 68.897 | 1.00 15.61 | 7 | 3630 | O   | SER A 456 | 28.322 | 50.199 | 68.220 | 1.00 20.53 | 8 |
| 3594 | CA  | THR A 450  | 26.481 | 63.264 | 67.761 | 1.00 13.97 | 6 | 3631 | CB  | SER A 456 | 29.916 | 49.747 | 70.778 | 1.00 22.39 | 6 |
| 3595 | C   | THR A 450  | 24.998 | 63.001 | 67.994 | 1.00 16.43 | 6 | 3632 | OG  | SER A 456 | 30.178 | 49.998 | 72.161 | 1.00 30.42 | 8 |
| 3596 | O   | THR A 450  | 24.528 | 62.925 | 69.160 | 1.00 16.61 | 8 | 3633 | N   | TYR A 457 | 30.024 | 51.683 | 68.013 | 1.00 15.08 | 7 |
| 3597 | CB  | THR A 450  | 27.216 | 61.912 | 67.566 | 1.00 15.00 | 6 | 3634 | CA  | TYR A 457 | 29.941 | 51.627 | 66.559 | 1.00 13.18 | 6 |
| 3598 | OG1 | THR A 450  | 26.686 | 61.176 | 66.471 | 1.00 15.07 | 8 | 3635 | C   | TYR A 457 | 31.301 | 51.229 | 65.961 | 1.00 14.20 | 6 |
| 3599 | CG2 | THR A 450  | 27.007 | 61.016 | 68.814 | 1.00 18.27 | 6 | 3636 | O   | TYR A 457 | 32.257 | 51.915 | 66.259 | 1.00 16.66 | 8 |
| 3599 | N   | ALA A 451  | 24.286 | 62.806 | 66.886 | 1.00 15.10 | 7 | 3637 | CB  | TYR A 457 | 29.564 | 53.017 | 65.941 | 1.00 17.47 | 6 |

|      |     |     |   |     |        |        |        |      |       |   |      |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 3638 | CG  | TYR | A | 457 | 28.122 | 53.387 | 66.241 | 1.00 | 15.26 | 6 | 3680 | C   | SER | A | 462 | 38.011 | 48.422 | 58.907 | 1.00 | 17.10 | 6 |
| 3639 | CD1 | TYR | A | 457 | 27.799 | 53.933 | 67.497 | 1.00 | 15.37 | 6 | 3681 | O   | SER | A | 462 | 38.878 | 47.546 | 58.763 | 1.00 | 16.40 | 8 |
| 3640 | CD2 | TYR | A | 457 | 27.077 | 53.174 | 65.325 | 1.00 | 16.16 | 6 | 3682 | CB  | SER | A | 462 | 36.316 | 46.813 | 57.987 | 1.00 | 19.17 | 6 |
| 3641 | CE1 | TYR | A | 457 | 26.521 | 54.297 | 67.873 | 1.00 | 15.82 | 6 | 3683 | OG  | SER | A | 462 | 34.914 | 46.479 | 57.974 | 1.00 | 20.76 | 8 |
| 3642 | CE2 | TYR | A | 457 | 25.768 | 53.516 | 65.671 | 1.00 | 15.99 | 6 | 3684 | N   | GLY | A | 463 | 38.369 | 49.689 | 59.115 | 1.00 | 13.98 | 7 |
| 3643 | CZ  | TYR | A | 457 | 25.523 | 54.070 | 66.928 | 1.00 | 16.37 | 6 | 3685 | CA  | GLY | A | 463 | 39.781 | 50.089 | 59.271 | 1.00 | 14.97 | 6 |
| 3644 | OH  | TYR | A | 457 | 24.210 | 54.401 | 67.218 | 1.00 | 16.11 | 8 | 3686 | C   | GLY | A | 463 | 40.533 | 50.140 | 57.949 | 1.00 | 15.42 | 6 |
| 3645 | N   | ALA | A | 458 | 31.329 | 50.211 | 65.128 | 1.00 | 14.59 | 7 | 3687 | O   | GLY | A | 463 | 41.745 | 50.387 | 57.984 | 1.00 | 15.84 | 8 |
| 3646 | CA  | ALA | A | 458 | 32.601 | 49.943 | 64.445 | 1.00 | 17.03 | 6 | 3688 | N   | LEU | A | 464 | 39.816 | 50.043 | 56.808 | 1.00 | 12.86 | 7 |
| 3647 | C   | ALA | A | 458 | 32.686 | 50.915 | 63.247 | 1.00 | 14.66 | 6 | 3689 | CA  | LEU | A | 464 | 40.559 | 50.113 | 55.525 | 1.00 | 10.93 | 6 |
| 3648 | O   | ALA | A | 458 | 31.654 | 51.326 | 62.731 | 1.00 | 14.84 | 8 | 3690 | C   | LEU | A | 464 | 41.370 | 51.420 | 55.427 | 1.00 | 12.62 | 6 |
| 3649 | CB  | ALA | A | 458 | 32.638 | 48.538 | 63.857 | 1.00 | 17.50 | 6 | 3691 | O   | LEU | A | 464 | 42.484 | 51.408 | 54.854 | 1.00 | 14.36 | 8 |
| 3650 | N   | ASP | A | 459 | 33.942 | 51.128 | 62.831 | 1.00 | 13.42 | 7 | 3692 | CB  | LEU | A | 464 | 39.487 | 50.148 | 54.402 | 1.00 | 13.24 | 6 |
| 3651 | CA  | ASP | A | 459 | 34.082 | 51.858 | 61.521 | 1.00 | 11.91 | 6 | 3693 | CG  | LEU | A | 464 | 40.083 | 50.223 | 52.969 | 1.00 | 14.42 | 6 |
| 3652 | C   | ASP | A | 459 | 33.472 | 51.048 | 60.410 | 1.00 | 12.75 | 6 | 3694 | CD1 | LEU | A | 464 | 40.800 | 48.892 | 52.620 | 1.00 | 15.93 | 6 |
| 3653 | O   | ASP | A | 459 | 33.679 | 49.834 | 60.222 | 1.00 | 13.42 | 8 | 3695 | CD2 | LEU | A | 464 | 38.971 | 50.469 | 51.967 | 1.00 | 14.00 | 6 |
| 3654 | CB  | ASP | A | 459 | 35.567 | 52.007 | 61.258 | 1.00 | 12.66 | 6 | 3696 | N   | LEU | A | 465 | 40.797 | 52.526 | 55.872 | 1.00 | 11.79 | 7 |
| 3655 | CG  | ASP | A | 459 | 35.984 | 52.522 | 59.876 | 1.00 | 13.56 | 6 | 3697 | CA  | LEU | A | 465 | 41.473 | 53.824 | 55.761 | 1.00 | 12.51 | 6 |
| 3656 | OD1 | ASP | A | 459 | 35.143 | 53.232 | 59.328 | 1.00 | 12.36 | 8 | 3698 | C   | LEU | A | 465 | 41.953 | 54.319 | 57.114 | 1.00 | 13.32 | 6 |
| 3657 | OD2 | ASP | A | 459 | 37.109 | 52.170 | 59.441 | 1.00 | 14.11 | 8 | 3699 | O   | LEU | A | 465 | 41.873 | 55.518 | 57.401 | 1.00 | 16.12 | 8 |
| 3658 | N   | TYR | A | 460 | 32.581 | 51.730 | 59.662 | 1.00 | 11.96 | 7 | 3700 | CB  | LEU | A | 465 | 40.510 | 54.894 | 55.130 | 1.00 | 12.90 | 6 |
| 3659 | CA  | TYR | A | 460 | 31.927 | 51.022 | 58.513 | 1.00 | 13.29 | 6 | 3701 | CG  | LEU | A | 465 | 40.090 | 54.441 | 53.714 | 1.00 | 12.88 | 6 |
| 3660 | C   | TYR | A | 460 | 32.905 | 50.541 | 57.467 | 1.00 | 16.04 | 6 | 3702 | CD1 | LEU | A | 465 | 39.162 | 55.509 | 53.111 | 1.00 | 14.96 | 6 |
| 3661 | O   | TYR | A | 460 | 32.617 | 49.627 | 56.683 | 1.00 | 15.32 | 8 | 3703 | CD2 | LEU | A | 465 | 41.263 | 54.191 | 52.777 | 1.00 | 14.83 | 6 |
| 3662 | CB  | TYR | A | 460 | 30.909 | 52.021 | 57.931 | 1.00 | 13.60 | 6 | 3704 | N   | GLY | A | 466 | 42.237 | 53.348 | 58.043 | 1.00 | 14.06 | 7 |
| 3663 | CG  | TYR | A | 460 | 29.970 | 51.418 | 56.899 | 1.00 | 13.06 | 6 | 3705 | CA  | GLY | A | 466 | 42.789 | 53.800 | 59.336 | 1.00 | 14.74 | 6 |
| 3664 | CD1 | TYR | A | 460 | 28.809 | 50.815 | 57.400 | 1.00 | 11.63 | 6 | 3706 | C   | GLY | A | 466 | 41.735 | 54.095 | 60.400 | 1.00 | 14.06 | 6 |
| 3665 | CD2 | TYR | A | 460 | 30.215 | 51.365 | 55.532 | 1.00 | 16.49 | 6 | 3707 | O   | GLY | A | 466 | 42.061 | 54.643 | 61.479 | 1.00 | 15.13 | 8 |
| 3666 | CE1 | TYR | A | 460 | 27.838 | 50.274 | 56.514 | 1.00 | 15.86 | 6 | 3708 | N   | GLY | A | 467 | 40.451 | 53.817 | 60.125 | 1.00 | 13.86 | 7 |
| 3667 | CE2 | TYR | A | 460 | 29.278 | 50.783 | 54.562 | 1.00 | 15.66 | 6 | 3709 | CA  | GLY | A | 467 | 39.357 | 54.137 | 61.045 | 1.00 | 11.80 | 6 |
| 3668 | CZ  | TYR | A | 460 | 28.098 | 50.257 | 55.165 | 1.00 | 17.45 | 6 | 3710 | C   | GLY | A | 467 | 39.321 | 53.244 | 62.311 | 1.00 | 14.35 | 6 |
| 3669 | OH  | TYR | A | 460 | 27.209 | 49.696 | 54.262 | 1.00 | 16.44 | 8 | 3711 | O   | GLY | A | 467 | 40.083 | 52.261 | 62.394 | 1.00 | 16.59 | 8 |
| 3670 | N   | LEU | A | 461 | 34.057 | 51.242 | 57.374 | 1.00 | 13.04 | 7 | 3712 | N   | ASN | A | 468 | 38.509 | 53.696 | 63.236 | 1.00 | 15.29 | 7 |
| 3671 | CA  | LEU | A | 461 | 35.137 | 50.814 | 56.424 | 1.00 | 13.89 | 6 | 3713 | CA  | ASN | A | 468 | 38.483 | 53.050 | 64.569 | 1.00 | 14.61 | 6 |
| 3672 | C   | LEU | A | 461 | 36.026 | 49.742 | 57.023 | 1.00 | 14.71 | 6 | 3714 | C   | ASN | A | 468 | 37.007 | 52.960 | 64.963 | 1.00 | 15.14 | 6 |
| 3673 | O   | LEU | A | 461 | 36.992 | 49.331 | 56.369 | 1.00 | 13.39 | 8 | 3715 | O   | ASN | A | 468 | 36.145 | 53.679 | 64.418 | 1.00 | 15.07 | 8 |
| 3674 | CB  | LEU | A | 461 | 35.968 | 52.115 | 56.171 | 1.00 | 13.08 | 6 | 3716 | CB  | ASN | A | 468 | 39.253 | 54.012 | 65.515 | 1.00 | 16.45 | 6 |
| 3675 | CG  | LEU | A | 461 | 35.299 | 53.075 | 55.149 | 1.00 | 13.44 | 6 | 3717 | CG  | ASN | A | 468 | 38.730 | 55.429 | 65.538 | 1.00 | 17.15 | 6 |
| 3676 | CD1 | LEU | A | 461 | 35.968 | 54.453 | 55.284 | 1.00 | 14.44 | 6 | 3718 | OD1 | ASN | A | 468 | 39.013 | 56.375 | 64.739 | 1.00 | 19.92 | 8 |
| 3677 | CD2 | LEU | A | 461 | 35.485 | 52.526 | 53.743 | 1.00 | 16.37 | 6 | 3719 | ND2 | ASN | A | 468 | 37.812 | 55.710 | 66.490 | 1.00 | 16.39 | 7 |
| 3678 | N   | SER | A | 462 | 35.746 | 49.218 | 58.222 | 1.00 | 15.11 | 7 | 3720 | N   | GLY | A | 469 | 36.787 | 52.285 | 66.076 | 1.00 | 16.49 | 7 |
| 3679 | CA  | SER | A | 462 | 36.521 | 48.122 | 58.810 | 1.00 | 16.17 | 6 | 3721 | CA  | GLY | A | 469 | 35.415 | 52.189 | 66.624 | 1.00 | 16.85 | 6 |



|      |     |     |   |     |        |        |        |      |       |   |      |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 3804 | CG2 | THR | A | 481 | 44.953 | 58.894 | 68.091 | 1.00 | 20.55 | 6 | 3846 | OG  | SER | A | 488 | 36.431 | 55.439 | 61.907 | 1.00 | 19.75 | 8 |
| 3805 | N   | LEU | A | 482 | 42.216 | 59.860 | 66.454 | 1.00 | 14.98 | 7 | 3847 | N   | VAL | A | 489 | 33.950 | 55.975 | 59.626 | 1.00 | 11.85 | 7 |
| 3806 | CA  | LEU | A | 482 | 42.004 | 59.690 | 64.991 | 1.00 | 13.06 | 6 | 3848 | CA  | VAL | A | 489 | 32.567 | 56.313 | 59.340 | 1.00 | 11.74 | 6 |
| 3807 | C   | LEU | A | 482 | 43.383 | 59.527 | 64.394 | 1.00 | 14.32 | 6 | 3849 | C   | VAL | A | 489 | 31.685 | 55.457 | 60.269 | 1.00 | 12.51 | 6 |
| 3808 | O   | LEU | A | 482 | 44.199 | 60.432 | 64.487 | 1.00 | 15.20 | 8 | 3850 | O   | VAL | A | 489 | 31.910 | 54.276 | 60.410 | 1.00 | 13.59 | 8 |
| 3809 | CB  | LEU | A | 482 | 41.231 | 60.917 | 64.486 | 1.00 | 13.14 | 6 | 3851 | CB  | VAL | A | 489 | 32.231 | 55.903 | 57.882 | 1.00 | 12.50 | 6 |
| 3810 | CG  | LEU | A | 482 | 40.812 | 60.936 | 62.999 | 1.00 | 14.96 | 6 | 3852 | CG1 | VAL | A | 489 | 30.712 | 56.154 | 57.650 | 1.00 | 11.14 | 6 |
| 3811 | CD1 | LEU | A | 482 | 39.938 | 59.717 | 62.720 | 1.00 | 16.24 | 6 | 3853 | CG2 | VAL | A | 489 | 32.978 | 56.812 | 56.882 | 1.00 | 13.14 | 6 |
| 3812 | CD2 | LEU | A | 482 | 40.073 | 62.242 | 62.727 | 1.00 | 14.36 | 6 | 3854 | N   | TRP | A | 490 | 30.771 | 56.135 | 60.914 | 1.00 | 11.35 | 7 |
| 3813 | N   | ALA | A | 483 | 43.621 | 58.414 | 63.680 | 1.00 | 12.65 | 7 | 3855 | CA  | TRP | A | 490 | 29.900 | 55.413 | 61.883 | 1.00 | 11.90 | 6 |
| 3814 | CA  | ALA | A | 483 | 44.961 | 58.090 | 63.175 | 1.00 | 13.54 | 6 | 3856 | C   | TRP | A | 490 | 28.446 | 55.715 | 61.508 | 1.00 | 13.16 | 6 |
| 3815 | C   | ALA | A | 483 | 45.370 | 58.961 | 62.000 | 1.00 | 13.15 | 6 | 3857 | O   | TRP | A | 490 | 28.103 | 56.878 | 61.324 | 1.00 | 16.40 | 8 |
| 3816 | O   | ALA | A | 483 | 44.562 | 59.723 | 61.387 | 1.00 | 13.10 | 8 | 3858 | CB  | TRP | A | 490 | 30.222 | 55.953 | 63.283 | 1.00 | 12.61 | 6 |
| 3817 | CB  | ALA | A | 483 | 44.892 | 56.581 | 62.782 | 1.00 | 12.82 | 6 | 3859 | CG  | TRP | A | 490 | 31.708 | 55.807 | 63.639 | 1.00 | 12.91 | 6 |
| 3818 | N   | PRO | A | 484 | 46.637 | 58.980 | 61.687 | 1.00 | 14.66 | 7 | 3860 | CD1 | TRP | A | 490 | 32.381 | 54.628 | 63.904 | 1.00 | 14.71 | 6 |
| 3819 | CA  | PRO | A | 484 | 47.183 | 59.827 | 60.632 | 1.00 | 11.27 | 6 | 3861 | CD2 | TRP | A | 490 | 32.632 | 56.884 | 63.716 | 1.00 | 14.18 | 6 |
| 3820 | C   | PRO | A | 484 | 46.509 | 59.496 | 59.301 | 1.00 | 12.98 | 6 | 3862 | NE1 | TRP | A | 490 | 33.717 | 54.969 | 64.166 | 1.00 | 13.76 | 7 |
| 3821 | O   | PRO | A | 484 | 46.374 | 58.331 | 58.884 | 1.00 | 13.40 | 8 | 3863 | CE2 | TRP | A | 490 | 33.883 | 56.328 | 64.049 | 1.00 | 14.41 | 6 |
| 3822 | CB  | PRO | A | 484 | 48.704 | 59.546 | 60.545 | 1.00 | 15.48 | 6 | 3864 | CE3 | TRP | A | 490 | 32.509 | 58.271 | 63.546 | 1.00 | 16.82 | 6 |
| 3823 | CG  | PRO | A | 484 | 48.959 | 58.945 | 61.936 | 1.00 | 15.92 | 6 | 3865 | CZ2 | TRP | A | 490 | 35.020 | 57.117 | 64.216 | 1.00 | 13.91 | 6 |
| 3824 | CD  | PRO | A | 484 | 47.698 | 58.160 | 62.333 | 1.00 | 15.61 | 6 | 3866 | CZ3 | TRP | A | 490 | 33.641 | 59.052 | 63.701 | 1.00 | 14.61 | 6 |
| 3825 | N   | GLY | A | 485 | 45.977 | 60.548 | 58.671 | 1.00 | 14.03 | 7 | 3867 | CH2 | TRP | A | 490 | 34.894 | 58.461 | 64.044 | 1.00 | 14.54 | 6 |
| 3826 | CA  | GLY | A | 485 | 45.399 | 60.352 | 57.309 | 1.00 | 13.19 | 6 | 3868 | N   | GLN | A | 491 | 27.680 | 54.618 | 61.394 | 1.00 | 11.75 | 7 |
| 3827 | C   | GLY | A | 485 | 44.067 | 59.600 | 57.376 | 1.00 | 16.21 | 6 | 3869 | CA  | GLN | A | 491 | 26.332 | 54.869 | 60.903 | 1.00 | 12.20 | 6 |
| 3828 | O   | GLY | A | 485 | 43.561 | 59.235 | 56.271 | 1.00 | 13.21 | 8 | 3870 | C   | GLN | A | 491 | 25.221 | 54.121 | 61.637 | 1.00 | 13.63 | 6 |
| 3829 | N   | ALA | A | 486 | 43.508 | 59.349 | 58.553 | 1.00 | 11.65 | 7 | 3871 | O   | GLN | A | 491 | 25.472 | 53.092 | 62.207 | 1.00 | 13.45 | 8 |
| 3830 | CA  | ALA | A | 486 | 42.375 | 58.395 | 58.545 | 1.00 | 13.98 | 6 | 3872 | CB  | GLN | A | 491 | 26.259 | 54.452 | 59.410 | 1.00 | 12.17 | 6 |
| 3831 | C   | ALA | A | 486 | 41.058 | 58.969 | 58.068 | 1.00 | 15.41 | 6 | 3873 | CG  | GLN | A | 491 | 26.541 | 52.972 | 59.117 | 1.00 | 12.78 | 6 |
| 3832 | O   | ALA | A | 486 | 40.730 | 60.148 | 58.196 | 1.00 | 13.33 | 8 | 3874 | CD  | GLN | A | 491 | 25.208 | 52.219 | 58.993 | 1.00 | 19.79 | 6 |
| 3833 | CB  | ALA | A | 486 | 42.233 | 57.937 | 60.002 | 1.00 | 14.43 | 6 | 3875 | OE1 | GLN | A | 491 | 24.222 | 52.726 | 58.485 | 1.00 | 16.61 | 8 |
| 3834 | N   | VAL | A | 487 | 40.213 | 58.008 | 57.647 | 1.00 | 12.17 | 7 | 3876 | NE2 | GLN | A | 491 | 25.214 | 50.952 | 59.455 | 1.00 | 19.28 | 7 |
| 3835 | CA  | VAL | A | 487 | 38.776 | 58.220 | 57.403 | 1.00 | 9.79  | 6 | 3877 | N   | TYR | A | 492 | 24.024 | 54.698 | 61.523 | 1.00 | 13.67 | 7 |
| 3836 | C   | VAL | A | 487 | 38.057 | 57.174 | 58.257 | 1.00 | 9.96  | 6 | 3878 | CA  | TYR | A | 492 | 22.819 | 54.043 | 62.092 | 1.00 | 14.21 | 6 |
| 3837 | O   | VAL | A | 487 | 38.406 | 55.970 | 58.179 | 1.00 | 12.30 | 8 | 3879 | C   | TYR | A | 492 | 21.665 | 54.203 | 61.102 | 1.00 | 17.30 | 6 |
| 3838 | CB  | VAL | A | 487 | 38.428 | 58.022 | 55.919 | 1.00 | 10.95 | 6 | 3880 | O   | TYR | A | 492 | 21.507 | 55.341 | 60.614 | 1.00 | 14.76 | 8 |
| 3839 | CG1 | VAL | A | 487 | 36.871 | 58.150 | 55.762 | 1.00 | 12.89 | 6 | 3881 | CB  | TYR | A | 492 | 22.452 | 54.774 | 63.393 | 1.00 | 15.27 | 6 |
| 3840 | CG2 | VAL | A | 487 | 39.127 | 58.990 | 54.964 | 1.00 | 15.13 | 6 | 3882 | CG  | TYR | A | 492 | 21.152 | 54.219 | 63.984 | 1.00 | 15.56 | 6 |
| 3841 | N   | SER | A | 488 | 37.112 | 57.635 | 59.078 | 1.00 | 11.84 | 7 | 3883 | CD1 | TYR | A | 492 | 21.146 | 53.010 | 64.638 | 1.00 | 20.95 | 6 |
| 3842 | CA  | SER | A | 488 | 36.335 | 56.623 | 59.865 | 1.00 | 12.18 | 6 | 3884 | CD2 | TYR | A | 492 | 19.963 | 54.959 | 63.800 | 1.00 | 18.48 | 6 |
| 3843 | C   | SER | A | 488 | 34.867 | 56.972 | 59.699 | 1.00 | 11.64 | 6 | 3885 | CE1 | TYR | A | 492 | 19.956 | 52.511 | 65.176 | 1.00 | 21.55 | 6 |
| 3844 | O   | SER | A | 488 | 34.519 | 58.154 | 59.650 | 1.00 | 12.81 | 8 | 3886 | CE2 | TYR | A | 492 | 18.770 | 54.444 | 64.324 | 1.00 | 19.51 | 6 |
| 3845 | CB  | SER | A | 488 | 36.850 | 56.705 | 61.336 | 1.00 | 15.82 | 6 | 3887 | CZ  | TYR | A | 492 | 18.817 | 53.254 | 65.003 | 1.00 | 22.52 | 6 |

|      |     |            |        |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|------------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3888 | OH  | TYR A 492  | 17.596 | 52.781 | 65.511 | 1.00 | 24.89 | 8 | 3928 | CB  | PRO A 499 | 4.930  | 59.294 | 54.823 | 1.00 | 20.07 | 6 |
| 3889 | N   | SER A 493  | 20.879 | 53.151 | 60.925 | 1.00 | 15.17 | 7 | 3929 | CG  | PRO A 499 | 3.927  | 59.790 | 55.829 | 1.00 | 23.72 | 6 |
| 3890 | CA  | SER A 493  | 19.666 | 53.363 | 60.096 | 1.00 | 14.91 | 6 | 3930 | CD  | PRO A 499 | 4.205  | 59.113 | 57.173 | 1.00 | 23.70 | 6 |
| 3891 | C   | SER A 493  | 18.548 | 52.462 | 60.616 | 1.00 | 20.17 | 6 | 3931 | N   | GLN A 500 | 8.288  | 59.975 | 55.037 | 1.00 | 18.24 | 7 |
| 3892 | O   | SER A 493  | 18.887 | 51.457 | 61.265 | 1.00 | 22.90 | 8 | 3932 | CA  | GLN A 500 | 9.423  | 60.939 | 55.075 | 1.00 | 13.65 | 6 |
| 3893 | CB  | SER A 493  | 19.867 | 53.083 | 58.619 | 1.00 | 23.97 | 6 | 3933 | C   | GLN A 500 | 9.921  | 61.084 | 53.596 | 1.00 | 12.93 | 6 |
| 3894 | OG  | SER A 493  | 20.148 | 51.710 | 58.532 | 1.00 | 30.62 | 8 | 3934 | O   | GLN A 500 | 10.256 | 60.065 | 53.014 | 1.00 | 15.78 | 8 |
| 3895 | N   | THR A 494  | 17.344 | 52.991 | 60.393 | 1.00 | 15.89 | 7 | 3935 | CB  | GLN A 500 | 10.601 | 60.286 | 55.860 | 1.00 | 15.18 | 6 |
| 3896 | CA  | THR A 494  | 16.243 | 52.127 | 60.906 | 1.00 | 18.40 | 6 | 3936 | CG  | GLN A 500 | 10.189 | 60.048 | 57.328 | 1.00 | 16.32 | 6 |
| 3897 | C   | THR A 494  | 14.999 | 52.406 | 60.060 | 1.00 | 20.14 | 6 | 3937 | CD  | GLN A 500 | 11.284 | 59.264 | 58.126 | 1.00 | 15.95 | 6 |
| 3898 | O   | THR A 494  | 14.967 | 53.429 | 59.367 | 1.00 | 20.45 | 8 | 3938 | OE1 | GLN A 500 | 12.239 | 58.781 | 57.571 | 1.00 | 17.99 | 8 |
| 3899 | CB  | THR A 494  | 15.993 | 52.424 | 62.396 | 1.00 | 24.38 | 6 | 3939 | NE2 | GLN A 500 | 11.008 | 59.238 | 59.419 | 1.00 | 20.52 | 7 |
| 3900 | OG1 | THR A 494  | 15.137 | 51.363 | 62.864 | 1.00 | 25.66 | 8 | 3940 | N   | ILE A 501 | 9.662  | 62.283 | 53.054 | 1.00 | 12.81 | 7 |
| 3901 | CG2 | THR A 494  | 15.368 | 53.751 | 62.737 | 1.00 | 27.09 | 6 | 3941 | CA  | ILE A 501 | 10.101 | 62.501 | 51.667 | 1.00 | 12.56 | 6 |
| 3902 | N   | SER A 495  | 14.017 | 51.534 | 60.157 | 1.00 | 22.56 | 7 | 3942 | C   | ILE A 501 | 11.594 | 62.914 | 51.642 | 1.00 | 13.47 | 6 |
| 3903 | CA  | SER A 495  | 12.772 | 51.870 | 59.422 | 1.00 | 19.72 | 6 | 3943 | O   | ILE A 501 | 11.899 | 63.905 | 52.301 | 1.00 | 14.35 | 8 |
| 3904 | C   | SER A 495  | 12.082 | 53.049 | 60.021 | 1.00 | 19.50 | 6 | 3944 | CB  | ILE A 501 | 9.262  | 63.635 | 51.032 | 1.00 | 12.51 | 6 |
| 3905 | O   | SER A 495  | 12.132 | 53.418 | 61.188 | 1.00 | 21.11 | 8 | 3945 | CG1 | ILE A 501 | 7.788  | 63.216 | 50.842 | 1.00 | 14.81 | 6 |
| 3906 | CB  | ASER A 495 | 11.766 | 50.698 | 59.444 | 0.60 | 26.59 | 6 | 3946 | CG2 | ILE A 501 | 9.888  | 63.939 | 49.629 | 1.00 | 12.71 | 6 |
| 3907 | OG  | ASER A 495 | 12.447 | 49.487 | 59.259 | 0.60 | 31.40 | 8 | 3947 | CD1 | ILE A 501 | 6.897  | 64.308 | 50.244 | 1.00 | 15.70 | 6 |
| 3907 | CB  | BSER A 495 | 11.888 | 50.603 | 59.441 | 0.40 | 20.10 | 6 | 3948 | N   | GLY A 502 | 12.383 | 62.169 | 50.872 | 1.00 | 12.33 | 7 |
| 3908 | OG  | BSER A 495 | 11.922 | 50.184 | 60.798 | 0.40 | 20.04 | 8 | 3949 | CA  | GLY A 502 | 13.793 | 62.673 | 50.746 | 1.00 | 12.41 | 6 |
| 3908 | N   | ALA A 496  | 11.315 | 53.727 | 59.141 | 1.00 | 20.53 | 7 | 3950 | C   | GLY A 502 | 13.915 | 63.416 | 49.403 | 1.00 | 11.68 | 8 |
| 3909 | CA  | ALA A 496  | 10.529 | 54.893 | 59.493 | 1.00 | 21.55 | 6 | 3951 | O   | GLY A 502 | 14.806 | 64.300 | 49.332 | 1.00 | 12.18 | 8 |
| 3910 | C   | ALA A 496  | 9.094  | 54.492 | 59.960 | 1.00 | 24.11 | 6 | 3952 | N   | SER A 503 | 13.120 | 63.068 | 48.395 | 1.00 | 12.99 | 7 |
| 3911 | O   | ALA A 496  | 8.536  | 53.596 | 59.350 | 1.00 | 29.93 | 8 | 3953 | CA  | SER A 503 | 13.334 | 63.710 | 47.073 | 1.00 | 12.73 | 6 |
| 3912 | CB  | ALA A 496  | 10.354 | 55.717 | 58.189 | 1.00 | 22.92 | 6 | 3954 | C   | SER A 503 | 11.970 | 63.672 | 46.342 | 1.00 | 14.01 | 6 |
| 3913 | N   | SER A 497  | 8.599  | 55.279 | 60.902 | 1.00 | 26.84 | 7 | 3955 | O   | SER A 503 | 11.263 | 62.678 | 46.449 | 1.00 | 14.22 | 8 |
| 3914 | CA  | SER A 497  | 7.226  | 54.967 | 61.354 | 1.00 | 32.64 | 6 | 3956 | CB  | SER A 503 | 14.364 | 62.853 | 46.296 | 1.00 | 12.66 | 6 |
| 3915 | C   | SER A 497  | 6.242  | 56.009 | 60.853 | 1.00 | 31.20 | 6 | 3957 | OG  | SER A 503 | 14.467 | 63.267 | 44.940 | 1.00 | 12.94 | 8 |
| 3916 | O   | SER A 497  | 5.049  | 55.788 | 61.090 | 1.00 | 33.40 | 8 | 3958 | N   | VAL A 504 | 11.736 | 64.763 | 45.625 | 1.00 | 12.13 | 7 |
| 3917 | CB  | SER A 497  | 7.183  | 54.836 | 62.875 | 1.00 | 35.13 | 6 | 3959 | CA  | VAL A 504 | 10.738 | 64.716 | 44.521 | 1.00 | 11.27 | 6 |
| 3918 | OG  | SER A 497  | 7.578  | 56.030 | 63.515 | 1.00 | 39.06 | 8 | 3960 | C   | VAL A 504 | 11.521 | 65.159 | 43.243 | 1.00 | 11.68 | 6 |
| 3919 | N   | ALA A 498  | 6.685  | 56.920 | 59.967 | 1.00 | 25.21 | 7 | 3961 | O   | VAL A 504 | 12.287 | 66.121 | 43.321 | 1.00 | 11.43 | 8 |
| 3920 | CA  | ALA A 498  | 5.749  | 57.878 | 59.354 | 1.00 | 21.05 | 6 | 3962 | CB  | VAL A 504 | 9.614  | 65.700 | 44.790 | 1.00 | 12.52 | 6 |
| 3921 | C   | ALA A 498  | 6.350  | 58.189 | 57.975 | 1.00 | 22.00 | 6 | 3963 | CG1 | VAL A 504 | 8.670  | 65.766 | 43.563 | 1.00 | 15.49 | 6 |
| 3922 | O   | ALA A 498  | 7.541  | 57.907 | 57.763 | 1.00 | 18.25 | 8 | 3964 | CG2 | VAL A 504 | 8.740  | 65.263 | 46.021 | 1.00 | 12.38 | 6 |
| 3923 | CB  | ALA A 498  | 5.737  | 59.103 | 60.231 | 1.00 | 22.15 | 6 | 3965 | N   | ALA A 505 | 11.424 | 64.285 | 42.236 | 1.00 | 11.00 | 7 |
| 3924 | N   | PRO A 499  | 5.633  | 58.771 | 57.054 | 1.00 | 18.84 | 7 | 3966 | CA  | ALA A 505 | 12.174 | 64.595 | 41.003 | 1.00 | 10.56 | 6 |
| 3925 | CA  | PRO A 499  | 6.176  | 59.058 | 55.718 | 1.00 | 19.31 | 6 | 3967 | C   | ALA A 505 | 11.447 | 64.174 | 39.798 | 1.00 | 12.28 | 6 |
| 3926 | C   | PRO A 499  | 7.174  | 60.210 | 55.762 | 1.00 | 15.69 | 6 | 3968 | O   | ALA A 505 | 10.738 | 63.165 | 39.919 | 1.00 | 13.54 | 8 |
| 3927 | O   | PRO A 499  | 6.934  | 61.242 | 56.370 | 1.00 | 16.96 | 8 | 3969 | CB  | ALA A 505 | 13.567 | 63.894 | 41.072 | 1.00 | 11.90 | 6 |







|      |     |           |        |        |        |            |   |      |     |           |        |        |        |            |   |
|------|-----|-----------|--------|--------|--------|------------|---|------|-----|-----------|--------|--------|--------|------------|---|
| 4138 | CB  | THR A 530 | -1.954 | 66.621 | 48.090 | 1.00 15.93 | 6 | 4180 | CA  | THR A 537 | -3.151 | 60.043 | 40.489 | 1.00 15.38 | 6 |
| 4139 | OG1 | THR A 530 | -1.209 | 66.722 | 49.308 | 1.00 17.69 | 8 | 4181 | C   | THR A 537 | -1.865 | 59.242 | 40.679 | 1.00 19.21 | 6 |
| 4140 | CG2 | THR A 530 | -3.279 | 65.858 | 48.340 | 1.00 17.39 | 6 | 4182 | O   | THR A 537 | -0.823 | 59.697 | 40.166 | 1.00 19.02 | 8 |
| 4141 | N   | PHE A 531 | -0.395 | 67.691 | 45.569 | 1.00 14.04 | 7 | 4183 | CB  | THR A 537 | -3.564 | 59.955 | 38.998 | 1.00 18.90 | 6 |
| 4142 | CA  | PHE A 531 | 0.458  | 68.822 | 45.142 | 1.00 13.01 | 6 | 4184 | OG1 | THR A 537 | -4.828 | 60.651 | 38.950 | 1.00 19.30 | 8 |
| 4143 | C   | PHE A 531 | -0.344 | 70.073 | 45.496 | 1.00 15.03 | 6 | 4185 | CG2 | THR A 537 | -3.697 | 58.508 | 38.591 | 1.00 18.81 | 6 |
| 4144 | O   | PHE A 531 | -1.454 | 70.292 | 44.989 | 1.00 16.16 | 8 | 4186 | N   | VAL A 538 | -1.925 | 58.176 | 41.415 | 1.00 16.51 | 7 |
| 4145 | CB  | PHE A 531 | 0.659  | 68.823 | 43.604 | 1.00 13.87 | 6 | 4187 | CA  | VAL A 538 | -0.704 | 57.394 | 41.746 | 1.00 16.38 | 6 |
| 4146 | CG  | PHE A 531 | 1.611  | 67.777 | 43.040 | 1.00 13.21 | 6 | 4188 | C   | VAL A 538 | -0.516 | 56.415 | 40.613 | 1.00 18.34 | 6 |
| 4147 | CD1 | PHE A 531 | 1.438  | 66.431 | 43.191 | 1.00 14.34 | 6 | 4189 | O   | VAL A 538 | -0.896 | 56.665 | 43.080 | 1.00 17.97 | 6 |
| 4148 | CD2 | PHE A 531 | 2.662  | 68.228 | 42.240 | 1.00 14.96 | 6 | 4190 | CB  | VAL A 538 | 0.219  | 55.621 | 43.337 | 1.00 16.03 | 6 |
| 4149 | CE1 | PHE A 531 | 2.288  | 65.515 | 42.629 | 1.00 16.70 | 6 | 4191 | CG1 | VAL A 538 | -1.016 | 57.646 | 44.226 | 1.00 19.59 | 6 |
| 4150 | CE2 | PHE A 531 | 3.545  | 67.306 | 41.691 | 1.00 13.81 | 6 | 4192 | CG2 | VAL A 538 | 0.696  | 56.340 | 40.055 | 1.00 15.64 | 7 |
| 4151 | CZ  | PHE A 531 | 3.385  | 65.943 | 41.836 | 1.00 16.70 | 6 | 4193 | N   | LYS A 539 | 1.119  | 55.341 | 39.108 | 1.00 14.97 | 6 |
| 4152 | N   | GLY A 532 | 0.118  | 70.806 | 46.490 | 1.00 14.18 | 7 | 4194 | CA  | LYS A 539 | 1.626  | 54.044 | 39.732 | 1.00 17.57 | 6 |
| 4153 | CA  | GLY A 532 | -0.569 | 72.077 | 46.884 | 1.00 15.57 | 6 | 4195 | C   | LYS A 539 | 1.313  | 52.885 | 39.375 | 1.00 18.05 | 8 |
| 4154 | C   | GLY A 532 | -1.992 | 71.702 | 47.378 | 1.00 19.88 | 6 | 4196 | O   | LYS A 539 | 2.264  | 55.914 | 38.209 | 1.00 17.15 | 6 |
| 4155 | O   | GLY A 532 | -2.928 | 72.482 | 47.068 | 1.00 18.91 | 8 | 4197 | CB  | LYS A 539 | 2.814  | 54.859 | 37.246 | 1.00 20.63 | 6 |
| 4156 | N   | GLY A 533 | -2.193 | 70.510 | 47.921 | 1.00 17.41 | 7 | 4198 | CG  | LYS A 539 | 3.860  | 55.636 | 36.368 | 1.00 25.39 | 6 |
| 4157 | CA  | GLY A 533 | -3.524 | 70.089 | 48.400 | 1.00 18.31 | 6 | 4199 | CD  | LYS A 539 | 3.601  | 55.199 | 34.949 | 1.00 41.98 | 6 |
| 4158 | C   | GLY A 533 | -4.368 | 69.372 | 47.370 | 1.00 20.08 | 6 | 4200 | CE  | LYS A 539 | 4.369  | 53.976 | 34.672 | 1.00 30.47 | 7 |
| 4159 | O   | GLY A 533 | -5.463 | 68.817 | 47.637 | 1.00 19.31 | 8 | 4201 | NZ  | LYS A 539 | 2.424  | 54.212 | 40.787 | 1.00 15.53 | 7 |
| 4160 | N   | VAL A 534 | -3.923 | 69.391 | 46.097 | 1.00 16.06 | 7 | 4202 | N   | SER A 540 | 2.919  | 53.073 | 41.587 | 1.00 16.52 | 6 |
| 4161 | CA  | VAL A 534 | -4.592 | 68.721 | 44.999 | 1.00 15.11 | 6 | 4203 | CA  | SER A 540 | 3.231  | 53.502 | 42.999 | 1.00 17.69 | 6 |
| 4162 | C   | VAL A 534 | -4.197 | 67.275 | 44.894 | 1.00 15.67 | 6 | 4204 | O   | SER A 540 | 3.482  | 54.680 | 43.306 | 1.00 16.82 | 8 |
| 4163 | O   | VAL A 534 | -3.019 | 66.888 | 44.712 | 1.00 17.94 | 8 | 4205 | O   | SER A 540 | 4.136  | 52.424 | 40.903 | 1.00 20.58 | 6 |
| 4164 | CB  | VAL A 534 | -4.368 | 69.480 | 43.645 | 1.00 13.67 | 6 | 4206 | CB  | SER A 540 | 5.270  | 53.317 | 41.043 | 1.00 19.05 | 8 |
| 4165 | CG1 | VAL A 534 | -5.101 | 68.739 | 42.509 | 1.00 15.45 | 6 | 4207 | OG  | SER A 540 | 3.206  | 52.536 | 43.953 | 1.00 16.64 | 7 |
| 4166 | CG2 | VAL A 534 | -4.807 | 70.937 | 43.768 | 1.00 16.93 | 6 | 4208 | N   | TRP A 541 | 3.361  | 52.905 | 45.378 | 1.00 15.40 | 6 |
| 4167 | N   | THR A 535 | -5.185 | 66.334 | 44.967 | 1.00 13.93 | 7 | 4209 | CA  | TRP A 541 | 4.148  | 51.785 | 46.053 | 1.00 20.16 | 6 |
| 4168 | CA  | THR A 535 | -4.827 | 64.927 | 44.890 | 1.00 16.87 | 6 | 4210 | C   | TRP A 541 | 3.682  | 50.647 | 46.008 | 1.00 21.11 | 8 |
| 4169 | O   | THR A 535 | -4.271 | 64.521 | 43.536 | 1.00 20.28 | 6 | 4211 | O   | TRP A 541 | 2.034  | 53.084 | 46.101 | 1.00 17.49 | 6 |
| 4170 | C   | THR A 535 | -4.796 | 64.893 | 42.462 | 1.00 17.64 | 8 | 4212 | CB  | TRP A 541 | 2.124  | 53.605 | 47.502 | 1.00 15.27 | 6 |
| 4171 | CB  | THR A 535 | -6.065 | 64.042 | 45.192 | 1.00 20.23 | 6 | 4213 | CG  | TRP A 541 | 2.645  | 52.924 | 48.584 | 1.00 18.64 | 6 |
| 4172 | OG1 | THR A 535 | -6.446 | 64.284 | 46.576 | 1.00 20.94 | 8 | 4214 | CD1 | TRP A 541 | 1.689  | 54.854 | 48.006 | 1.00 15.30 | 6 |
| 4173 | CG2 | THR A 535 | -5.787 | 62.565 | 45.026 | 1.00 24.73 | 6 | 4215 | CD2 | TRP A 541 | 2.542  | 53.673 | 49.715 | 1.00 19.85 | 7 |
| 4174 | N   | ALA A 536 | -3.162 | 63.773 | 43.562 | 1.00 15.87 | 7 | 4216 | NE1 | TRP A 541 | 1.976  | 54.894 | 49.381 | 1.00 17.27 | 6 |
| 4175 | CA  | ALA A 536 | -2.521 | 63.324 | 42.337 | 1.00 17.27 | 6 | 4217 | CE2 | TRP A 541 | 1.086  | 55.984 | 47.440 | 1.00 15.92 | 6 |
| 4176 | C   | ALA A 536 | -2.808 | 61.859 | 42.042 | 1.00 20.29 | 6 | 4218 | CE3 | TRP A 541 | 1.703  | 55.983 | 50.201 | 1.00 18.49 | 6 |
| 4177 | O   | ALA A 536 | -2.929 | 61.111 | 43.030 | 1.00 20.32 | 8 | 4219 | CZ2 | TRP A 541 | 0.787  | 57.054 | 48.223 | 1.00 19.66 | 6 |
| 4178 | CB  | ALA A 536 | -0.976 | 63.441 | 42.384 | 1.00 17.03 | 6 | 4220 | CZ3 | TRP A 541 | 1.076  | 57.063 | 49.619 | 1.00 21.41 | 6 |
| 4179 | N   | THR A 537 | -2.937 | 61.461 | 40.791 | 1.00 16.03 | 7 | 4221 | CH2 | TRP A 541 |        |        |        |            |   |

|      |     |      |       |        |        |        |      |       |   |      |     |     |       |       |        |        |      |       |   |
|------|-----|------|-------|--------|--------|--------|------|-------|---|------|-----|-----|-------|-------|--------|--------|------|-------|---|
| 4222 | N   | THR  | A 542 | 5.297  | 52.107 | 46.615 | 1.00 | 18.77 | 7 | 4260 | CG2 | ILE | A 546 | 3.624 | 57.682 | 45.030 | 1.00 | 14.12 | 6 |
| 4223 | CA  | THR  | A 542 | 6.111  | 51.224 | 47.437 | 1.00 | 20.27 | 6 | 4261 | CD1 | ILE | A 546 | 4.473 | 57.773 | 48.119 | 1.00 | 13.44 | 6 |
| 4224 | C   | THR  | A 542 | 6.477  | 51.972 | 48.690 | 1.00 | 21.74 | 6 | 4262 | N   | GLU | A 547 | 5.424 | 56.777 | 42.400 | 1.00 | 14.74 | 7 |
| 4225 | O   | THR  | A 542 | 6.369  | 53.228 | 48.814 | 1.00 | 17.27 | 8 | 4263 | CA  | GLU | A 547 | 5.338 | 57.543 | 41.134 | 1.00 | 14.58 | 6 |
| 4226 | CB  | THR  | A 542 | 7.356  | 50.641 | 46.743 | 1.00 | 24.92 | 6 | 4264 | C   | GLU | A 547 | 3.943 | 58.116 | 40.945 | 1.00 | 15.30 | 6 |
| 4227 | OG1 | THR  | A 542 | 8.305  | 51.745 | 46.576 | 1.00 | 21.04 | 8 | 4265 | O   | GLU | A 547 | 2.977 | 57.405 | 41.270 | 1.00 | 15.50 | 8 |
| 4228 | CG2 | THR  | A 542 | 7.091  | 49.930 | 45.442 | 1.00 | 26.69 | 6 | 4266 | CB  | GLU | A 547 | 5.537 | 56.644 | 39.913 | 1.00 | 14.75 | 6 |
| 4229 | N   | SER  | A 543 | 7.123  | 51.252 | 49.648 | 1.00 | 18.34 | 7 | 4267 | CG  | GLU | A 547 | 6.987 | 56.074 | 39.890 | 1.00 | 17.63 | 6 |
| 4230 | CA  | SER  | A 543 | 7.474  | 51.808 | 50.923 | 1.00 | 18.96 | 6 | 4268 | CD  | GLU | A 547 | 7.105 | 55.058 | 38.781 | 1.00 | 21.54 | 6 |
| 4231 | C   | SER  | A 543 | 8.463  | 52.975 | 50.734 | 1.00 | 17.37 | 6 | 4269 | OE1 | GLU | A 547 | 6.335 | 54.046 | 38.730 | 1.00 | 18.28 | 8 |
| 4232 | O   | SER  | A 543 | 8.525  | 53.808 | 51.615 | 1.00 | 19.43 | 8 | 4270 | OE2 | GLU | A 547 | 7.924 | 55.225 | 37.834 | 1.00 | 16.92 | 8 |
| 4233 | CB  | SER  | A 543 | 8.201  | 50.711 | 51.743 | 1.00 | 24.79 | 6 | 4271 | N   | VAL | A 548 | 3.865 | 59.377 | 40.603 | 1.00 | 12.67 | 7 |
| 4234 | OG  | SER  | A 543 | 7.254  | 49.673 | 51.954 | 1.00 | 38.42 | 8 | 4272 | CA  | VAL | A 548 | 2.565 | 60.033 | 40.428 | 1.00 | 13.16 | 6 |
| 4235 | N   | ASN  | A 544 | 9.313  | 52.865 | 49.721 | 1.00 | 17.78 | 7 | 4273 | C   | VAL | A 548 | 2.565 | 60.764 | 39.095 | 1.00 | 15.52 | 6 |
| 4236 | CA  | ASN  | A 544 | 10.349 | 53.917 | 49.575 | 1.00 | 14.67 | 6 | 4274 | O   | VAL | A 548 | 3.587 | 61.028 | 38.477 | 1.00 | 14.55 | 8 |
| 4237 | C   | ASN  | A 544 | 10.208 | 54.723 | 48.287 | 1.00 | 15.24 | 6 | 4275 | CB  | VAL | A 548 | 2.266 | 61.100 | 41.499 | 1.00 | 15.22 | 6 |
| 4238 | O   | ASN  | A 544 | 11.018 | 55.668 | 48.072 | 1.00 | 16.63 | 8 | 4276 | CG1 | VAL | A 548 | 2.134 | 60.409 | 42.872 | 1.00 | 17.06 | 6 |
| 4239 | CB  | ASN  | A 544 | 11.734 | 53.252 | 49.583 | 0.50 | 18.64 | 6 | 4277 | CG2 | VAL | A 548 | 3.376 | 62.179 | 41.584 | 1.00 | 16.26 | 6 |
| 4240 | CG  | AASN | A 544 | 12.145 | 52.868 | 51.005 | 0.50 | 24.93 | 6 | 4278 | N   | TYR | A 549 | 1.338 | 61.119 | 38.644 | 1.00 | 12.92 | 7 |
| 4241 | OD1 | AASN | A 544 | 11.394 | 53.024 | 51.976 | 0.50 | 27.01 | 8 | 4279 | CA  | TYR | A 549 | 1.226 | 61.997 | 37.481 | 1.00 | 14.43 | 6 |
| 4242 | ND2 | AASN | A 544 | 13.359 | 52.364 | 51.118 | 0.50 | 19.54 | 7 | 4280 | C   | TYR | A 549 | 0.902 | 63.397 | 37.975 | 1.00 | 13.16 | 6 |
| 4243 | CB  | BASN | A 544 | 11.746 | 53.263 | 49.523 | 0.50 | 15.95 | 6 | 4281 | O   | TYR | A 549 | 0.223 | 63.571 | 39.016 | 1.00 | 14.84 | 8 |
| 4244 | CG  | BASN | A 544 | 11.998 | 52.552 | 50.860 | 0.50 | 20.57 | 6 | 4282 | CB  | TYR | A 549 | 0.000 | 61.611 | 36.605 | 1.00 | 1     |   |

|      |     |           |        |        |        |      |       |    |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4302 | CG  | PRO A 551 | -1.772 | 66.991 | 40.707 | 1.00 | 20.55 | 6  | 4344 | C   | THR A 558 | 4.469  | 72.927 | 45.741 | 1.00 | 16.19 | 6 |
| 4303 | CD  | PRO A 551 | -0.427 | 66.849 | 39.973 | 1.00 | 17.00 | 6  | 4345 | O   | THR A 558 | 5.520  | 72.402 | 45.379 | 1.00 | 16.82 | 8 |
| 4304 | NA  | ASN A 552 | -3.658 | 68.150 | 36.821 | 1.00 | 15.47 | 7  | 4346 | CB  | THR A 558 | 2.616  | 73.378 | 44.044 | 1.00 | 17.75 | 6 |
| 4305 | CA  | ASN A 552 | -4.017 | 69.248 | 35.941 | 1.00 | 15.18 | 6  | 4347 | OG1 | THR A 558 | 1.566  | 73.153 | 45.010 | 1.00 | 18.46 | 8 |
| 4306 | C   | ASN A 552 | -4.401 | 70.475 | 36.748 | 1.00 | 19.54 | 6  | 4348 | CG2 | THR A 558 | 2.886  | 72.099 | 43.320 | 1.00 | 14.65 | 6 |
| 4307 | O   | ASN A 552 | -5.630 | 70.744 | 36.917 | 1.00 | 19.65 | 8  | 4349 | N   | ASP A 559 | 3.750  | 72.559 | 46.821 | 1.00 | 13.53 | 7 |
| 4308 | CB  | ASN A 552 | -5.198 | 68.759 | 35.075 | 1.00 | 19.00 | 6  | 4350 | CA  | ASP A 559 | 4.351  | 71.569 | 47.739 | 1.00 | 13.26 | 6 |
| 4309 | CG  | ASN A 552 | -5.522 | 69.706 | 33.925 | 1.00 | 23.61 | 6  | 4351 | C   | ASP A 559 | 3.718  | 70.202 | 47.564 | 1.00 | 17.40 | 6 |
| 4310 | OD1 | ASN A 552 | -4.763 | 70.583 | 33.553 | 1.00 | 29.14 | 8  | 4352 | O   | ASP A 559 | 2.469  | 70.015 | 47.579 | 1.00 | 17.26 | 8 |
| 4311 | ND2 | ASN A 552 | -6.635 | 69.481 | 33.239 | 1.00 | 23.65 | 7  | 4353 | CB  | ASP A 559 | 4.129  | 72.027 | 49.195 | 1.00 | 13.77 | 6 |
| 4312 | N   | MET A 553 | -3.487 | 71.146 | 37.402 | 1.00 | 13.46 | 7  | 4354 | CG  | ASP A 559 | 4.998  | 73.219 | 49.580 | 1.00 | 25.94 | 6 |
| 4313 | CA  | MET A 553 | -3.722 | 72.208 | 38.346 | 1.00 | 11.50 | 6  | 4355 | OD1 | ASP A 559 | 6.174  | 73.267 | 49.201 | 1.00 | 23.88 | 8 |
| 4314 | C   | MET A 553 | -3.003 | 73.456 | 37.901 | 1.00 | 15.54 | 6  | 4356 | OD2 | ASP A 559 | 4.468  | 74.127 | 50.251 | 1.00 | 28.55 | 8 |
| 4315 | O   | MET A 553 | -2.319 | 73.427 | 36.881 | 1.00 | 17.61 | 8  | 4357 | N   | VAL A 560 | 4.576  | 69.205 | 47.465 | 1.00 | 12.44 | 7 |
| 4316 | CB  | MET A 553 | -3.328 | 71.835 | 39.803 | 1.00 | 16.46 | 6  | 4358 | CA  | VAL A 560 | 4.161  | 67.801 | 47.392 | 1.00 | 11.28 | 6 |
| 4317 | CG  | MET A 553 | -1.826 | 71.490 | 39.883 | 1.00 | 14.92 | 6  | 4359 | C   | VAL A 560 | 4.193  | 67.207 | 48.826 | 1.00 | 14.98 | 6 |
| 4318 | SD  | MET A 553 | -1.364 | 70.962 | 41.579 | 1.00 | 17.71 | 16 | 4360 | O   | VAL A 560 | 5.085  | 67.470 | 49.616 | 1.00 | 15.44 | 8 |
| 4319 | CE  | MET A 553 | -1.416 | 72.450 | 42.426 | 1.00 | 16.59 | 6  | 4361 | CB  | VAL A 560 | 5.144  | 66.953 | 46.555 | 1.00 | 11.93 | 6 |
| 4320 | N   | ALA A 554 | -3.278 | 74.532 | 38.619 | 1.00 | 17.19 | 7  | 4362 | CG1 | VAL A 560 | 4.738  | 65.496 | 46.488 | 1.00 | 16.58 | 6 |
| 4321 | CA  | ALA A 554 | -2.711 | 75.834 | 38.289 | 1.00 | 21.10 | 6  | 4363 | CG2 | VAL A 560 | 5.186  | 67.516 | 45.122 | 1.00 | 14.73 | 6 |
| 4322 | C   | ALA A 554 | -1.169 | 75.788 | 38.321 | 1.00 | 17.79 | 6  | 4364 | N   | LYS A 561 | 3.136  | 66.439 | 49.097 | 1.00 | 15.49 | 7 |
| 4323 | O   | ALA A 554 | -0.631 | 75.032 | 39.141 | 1.00 | 17.24 | 8  | 4365 | CA  | LYS A 561 | 2.989  | 65.835 | 50.443 | 1.00 | 14.90 | 6 |
| 4324 | CB  | ALA A 554 | -3.075 | 76.757 | 39.471 | 1.00 | 24.10 | 6  | 4366 | C   | LYS A 561 | 2.427  | 64.452 | 50.269 | 1.00 | 15.23 | 6 |
| 4325 | N   | ALA A 555 | -0.537 | 76.591 | 37.500 | 1.00 | 14.57 | 7  | 4367 | O   | LYS A 561 | 1.502  | 64.157 | 49.522 | 1.00 | 16.90 | 8 |
| 4326 | CA  | ALA A 555 | 0.947  | 76.567 | 37.489 | 1.00 | 13.27 | 6  | 4368 | CB  | LYS A 561 | 1.960  | 66.720 | 51.206 | 1.00 | 18.50 | 6 |
| 4327 | C   | ALA A 555 | 1.568  | 77.356 | 38.600 | 1.00 | 13.78 | 6  | 4369 | CG  | LYS A 561 | 1.847  | 66.177 | 52.656 | 1.00 | 22.42 | 6 |
| 4328 | O   | ALA A 555 | 1.051  | 78.305 | 39.204 | 1.00 | 14.85 | 8  | 4370 | CD  | LYS A 561 | 1.025  | 67.110 | 53.523 | 1.00 | 25.69 | 6 |
| 4329 | CB  | ALA A 555 | 1.375  | 77.200 | 36.142 | 1.00 | 16.26 | 6  | 4371 | CE  | LYS A 561 | -0.461 | 66.912 | 53.312 | 1.00 | 33.13 | 6 |
| 4330 | N   | GLY A 556 | 2.874  | 76.966 | 38.857 | 1.00 | 12.02 | 7  | 4372 | NZ  | LYS A 561 | -1.198 | 68.004 | 54.033 | 1.00 | 37.04 | 7 |
| 4331 | CA  | GLY A 556 | 3.602  | 77.675 | 39.947 | 1.00 | 14.17 | 6  | 4373 | N   | VAL A 562 | 2.947  | 63.489 | 51.047 | 1.00 | 16.07 | 7 |
| 4332 | C   | GLY A 556 | 4.312  | 76.639 | 40.815 | 1.00 | 12.79 | 6  | 4374 | CA  | VAL A 562 | 2.525  | 62.108 | 51.051 | 1.00 | 14.01 | 6 |
| 4333 | O   | GLY A 556 | 4.121  | 75.415 | 40.670 | 1.00 | 12.92 | 8  | 4375 | C   | VAL A 562 | 1.751  | 61.827 | 52.382 | 1.00 | 14.81 | 6 |
| 4334 | N   | LEU A 557 | 5.203  | 77.130 | 41.670 | 1.00 | 14.81 | 7  | 4376 | O   | VAL A 562 | 2.150  | 62.324 | 53.398 | 1.00 | 17.73 | 8 |
| 4335 | CA  | LEU A 557 | 5.876  | 76.232 | 42.626 | 1.00 | 13.54 | 6  | 4377 | CB  | VAL A 562 | 3.735  | 61.158 | 51.036 | 1.00 | 16.60 | 6 |
| 4336 | C   | LEU A 557 | 4.918  | 75.806 | 43.737 | 1.00 | 12.41 | 6  | 4378 | CG1 | VAL A 562 | 3.312  | 59.677 | 51.185 | 1.00 | 16.48 | 6 |
| 4337 | O   | LEU A 557 | 4.110  | 76.659 | 44.188 | 1.00 | 14.95 | 8  | 4379 | CG2 | VAL A 562 | 4.473  | 61.228 | 49.672 | 1.00 | 17.80 | 6 |
| 4338 | CB  | LEU A 557 | 7.091  | 76.999 | 43.221 | 1.00 | 13.41 | 6  | 4380 | N   | THR A 563 | 0.603  | 61.156 | 52.140 | 1.00 | 17.67 | 7 |
| 4339 | CG  | LEU A 557 | 8.018  | 76.123 | 44.069 | 1.00 | 15.11 | 6  | 4381 | CA  | THR A 563 | -0.181 | 60.806 | 53.380 | 1.00 | 18.18 | 6 |
| 4340 | CD1 | LEU A 557 | 8.847  | 75.220 | 43.141 | 1.00 | 13.33 | 6  | 4382 | C   | THR A 563 | -0.261 | 59.308 | 53.412 | 1.00 | 18.30 | 6 |
| 4341 | CD2 | LEU A 557 | 8.965  | 77.046 | 44.898 | 1.00 | 17.39 | 6  | 4383 | O   | THR A 563 | -0.679 | 58.642 | 52.456 | 1.00 | 19.93 | 8 |
| 4342 | N   | THR A 558 | 4.801  | 74.500 | 43.858 | 1.00 | 13.24 | 7  | 4384 | CB  | THR A 563 | -1.542 | 61.496 | 53.361 | 1.00 | 18.11 | 6 |
| 4343 | CA  | THR A 558 | 3.807  | 73.941 | 44.818 | 1.00 | 13.26 | 6  | 4385 | OG1 | THR A 563 | -1.367 | 62.891 | 53.406 | 1.00 | 19.44 | 8 |

|      |     |     |   |     |        |        |        |      |       |   |      |     |      |   |     |        |        |        |      |       |   |
|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|------|---|-----|--------|--------|--------|------|-------|---|
| 4386 | CG2 | THR | A | 563 | -2.281 | 61.112 | 54.705 | 1.00 | 20.36 | 6 | 4428 | CA  | LEU  | A | 571 | 6.705  | 68.878 | 52.131 | 1.00 | 12.49 | 6 |
| 4387 | N   | ALA | A | 564 | 0.154  | 58.701 | 54.548 | 1.00 | 21.05 | 7 | 4429 | C   | LEU  | A | 571 | 7.959  | 69.019 | 51.282 | 1.00 | 15.87 | 6 |
| 4388 | CA  | ALA | A | 564 | 0.245  | 57.258 | 54.649 | 1.00 | 24.26 | 6 | 4430 | O   | LEU  | A | 571 | 9.024  | 69.355 | 51.828 | 1.00 | 16.79 | 8 |
| 4389 | C   | ALA | A | 564 | -0.234 | 56.845 | 56.060 | 1.00 | 23.28 | 6 | 4431 | CB  | LEU  | A | 571 | 6.147  | 70.286 | 52.340 | 1.00 | 15.18 | 6 |
| 4390 | O   | ALA | A | 564 | 0.104  | 57.536 | 57.008 | 1.00 | 21.58 | 8 | 4432 | CG  | LEU  | A | 571 | 4.911  | 70.396 | 53.250 | 1.00 | 22.77 | 6 |
| 4391 | CB  | ALA | A | 564 | 1.658  | 56.711 | 54.437 | 1.00 | 25.03 | 6 | 4433 | CD1 | LEU  | A | 571 | 4.368  | 71.807 | 53.300 | 1.00 | 22.26 | 6 |
| 4392 | N   | GLY | A | 565 | -1.218 | 55.968 | 56.140 | 1.00 | 30.08 | 7 | 4434 | CD2 | LEU  | A | 571 | 3.834  | 69.448 | 52.757 | 1.00 | 22.04 | 6 |
| 4393 | CA  | GLY | A | 565 | -1.857 | 55.701 | 57.443 | 1.00 | 31.09 | 6 | 4435 | N   | TYR  | A | 572 | 7.747  | 68.878 | 49.946 | 1.00 | 13.65 | 7 |
| 4394 | C   | GLY | A | 565 | -2.488 | 56.887 | 58.121 | 1.00 | 35.06 | 6 | 4436 | CA  | TYR  | A | 572 | 8.930  | 69.100 | 49.067 | 1.00 | 12.87 | 6 |
| 4395 | O   | GLY | A | 565 | -2.493 | 56.983 | 59.363 | 1.00 | 31.36 | 8 | 4437 | C   | TYR  | A | 572 | 8.322  | 69.878 | 47.880 | 1.00 | 14.52 | 6 |
| 4396 | N   | GLY | A | 566 | -3.025 | 57.873 | 57.403 | 1.00 | 32.22 | 7 | 4438 | O   | TYR  | A | 572 | 7.347  | 69.399 | 47.262 | 1.00 | 14.71 | 8 |
| 4397 | CA  | GLY | A | 566 | -3.549 | 59.083 | 58.011 | 1.00 | 31.70 | 6 | 4439 | CB  | TYR  | A | 572 | 9.480  | 67.704 | 48.701 | 1.00 | 12.62 | 6 |
| 4398 | C   | GLY | A | 566 | -2.523 | 60.107 | 58.438 | 1.00 | 31.07 | 6 | 4440 | CG  | TYR  | A | 572 | 10.887 | 67.679 | 48.121 | 1.00 | 13.61 | 6 |
| 4399 | O   | GLY | A | 566 | -2.936 | 61.213 | 58.829 | 1.00 | 32.69 | 8 | 4441 | CD1 | TYR  | A | 572 | 11.079 | 68.175 | 46.835 | 1.00 | 13.57 | 6 |
| 4400 | N   | VAL | A | 567 | -1.202 | 59.887 | 58.271 | 1.00 | 26.17 | 7 | 4442 | CD2 | TYR  | A | 572 | 11.946 | 67.161 | 48.845 | 1.00 | 15.40 | 6 |
| 4401 | CA  | VAL | A | 567 | -0.186 | 60.798 | 58.776 | 1.00 | 21.45 | 6 | 4443 | CE1 | TYR  | A | 572 | 12.361 | 68.168 | 46.257 | 1.00 | 13.80 | 6 |
| 4402 | C   | VAL | A | 567 | 0.537  | 61.488 | 57.557 | 1.00 | 17.95 | 6 | 4444 | CE2 | TYR  | A | 572 | 13.221 | 67.135 | 48.283 | 1.00 | 12.70 | 6 |
| 4403 | O   | VAL | A | 567 | 0.692  | 60.707 | 56.658 | 1.00 | 18.75 | 8 | 4445 | CZ  | TYR  | A | 572 | 13.400 | 67.629 | 47.002 | 1.00 | 14.33 | 6 |
| 4404 | CB  | VAL | A | 567 | 0.945  | 60.023 | 59.500 | 1.00 | 26.89 | 6 | 4446 | OH  | TYR  | A | 572 | 14.710 | 67.607 | 46.466 | 1.00 | 13.40 | 8 |
| 4405 | CG1 | VAL | A | 567 | 1.981  | 60.946 | 60.096 | 1.00 | 30.00 | 6 | 4447 | N   | SER  | A | 573 | 9.060  | 70.874 | 47.387 | 1.00 | 13.37 | 7 |
| 4406 | CG2 | VAL | A | 567 | 0.308  | 59.088 | 60.567 | 1.00 | 33.86 | 6 | 4448 | CA  | SER  | A | 573 | 8.571  | 71.734 | 46.294 | 1.00 | 12.21 | 6 |
| 4407 | N   | SER | A | 568 | 0.687  | 62.774 | 57.699 | 1.00 | 19.77 | 7 | 4449 | C   | SER  | A | 573 | 8.665  | 71.055 | 44.920 | 1.00 | 12.75 | 6 |
| 4408 | CA  | SER | A | 568 | 1.267  | 63.410 | 56.486 | 1.00 | 19.16 | 6 | 4450 | O   | SER  | A | 573 | 9.520  | 70.234 | 44.703 | 1.00 | 12.64 | 8 |
| 4409 | C   | SER | A | 568 | 2.770  | 63.585 | 56.688 | 1.00 | 19.28 | 6 | 4451 | CB  | ASER | A | 573 | 9.436  | 72.999 | 46.162 | 0.60 | 17.33 | 6 |
| 4410 | O   | SER | A | 568 | 3.351  | 63.752 | 57.763 | 1.00 | 21.35 | 8 | 4452 | OG  | ASER | A | 573 | 9.459  | 73.767 | 47.331 | 0.60 | 22.77 | 8 |
| 4411 | CB  | SER | A | 568 | 0.574  | 64.705 | 56.156 | 1.00 | 29.69 | 6 | 4453 | CB  | BSER | A | 573 | 9.408  | 73.025 | 46.276 | 0.40 | 15.40 | 6 |
| 4412 | OG  | SER | A | 568 | 0.595  | 65.549 | 57.266 | 1.00 | 41.18 | 8 | 4454 | OG  | BSER | A | 573 | 10.793 | 72.728 | 46.149 | 0.40 | 16.17 | 8 |
| 4413 | N   | SER | A | 569 | 3.399  | 63.581 | 55.503 | 1.00 | 19.22 | 7 | 4455 | N   | TYR  | A | 574 | 7.838  | 71.568 | 44.000 | 1.00 | 11.56 | 7 |
| 4414 | CA  | SER | A | 569 | 4.867  | 63.784 | 55.480 | 1.00 | 17.43 | 6 | 4456 | CA  | TYR  | A | 574 | 7.912  | 71.077 | 42.604 | 1.00 | 10.89 | 6 |
| 4415 | C   | SER | A | 569 | 5.229  | 65.245 | 55.568 | 1.00 | 17.17 | 6 | 4457 | C   | TYR  | A | 574 | 7.374  | 72.249 | 41.771 | 1.00 | 13.28 | 6 |
| 4416 | O   | SER | A | 569 | 4.519  | 66.266 | 55.502 | 1.00 | 17.53 | 8 | 4458 | O   | TYR  | A | 574 | 6.344  | 72.860 | 42.138 | 1.00 | 12.17 | 8 |
| 4417 | CB  | SER | A | 569 | 5.381  | 63.220 | 54.137 | 1.00 | 17.58 | 6 | 4459 | CB  | TYR  | A | 574 | 7.041  | 69.857 | 42.405 | 1.00 | 11.94 | 6 |
| 4418 | OG  | SER | A | 569 | 5.066  | 64.083 | 53.025 | 1.00 | 15.50 | 8 | 4460 | CD1 | TYR  | A | 574 | 6.917  | 69.379 | 40.971 | 1.00 | 11.37 | 6 |
| 4419 | N   | ASN | A | 570 | 6.572  | 65.473 | 55.538 | 1.00 | 14.77 | 7 | 4461 | CD2 | TYR  | A | 574 | 7.921  | 68.521 | 40.467 | 1.00 | 12.69 | 6 |
| 4420 | CA  | ASN | A | 570 | 7.143  | 66.776 | 55.253 | 1.00 | 13.84 | 6 | 4462 | CE1 | TYR  | A | 574 | 5.867  | 69.781 | 40.162 | 1.00 | 11.85 | 6 |
| 4421 | C   | ASN | A | 570 | 6.848  | 67.107 | 53.752 | 1.00 | 13.33 | 6 | 4463 | CE2 | TYR  | A | 574 | 7.863  | 68.052 | 39.154 | 1.00 | 13.23 | 6 |
| 4422 | O   | ASN | A | 570 | 6.527  | 66.217 | 52.996 | 1.00 | 16.50 | 8 | 4464 | CZ  | TYR  | A | 574 | 5.792  | 69.313 | 38.834 | 1.00 | 13.93 | 6 |
| 4423 | CB  | ASN | A | 570 | 8.670  | 66.723 | 55.435 | 1.00 | 17.22 | 6 | 4465 | OH  | TYR  | A | 574 | 6.796  | 68.466 | 38.366 | 1.00 | 11.32 | 6 |
| 4424 | CG  | ASN | A | 570 | 9.363  | 65.581 | 54.758 | 1.00 | 16.95 | 6 | 4466 | N   | ASN  | A | 575 | 6.679  | 68.006 | 37.078 | 1.00 | 12.54 | 8 |
| 4425 | OD1 | ASN | A | 570 | 9.038  | 64.399 | 54.745 | 1.00 | 15.12 | 8 | 4467 | CA  | ASN  | A | 575 | 7.992  | 72.510 | 40.627 | 1.00 | 12.18 | 7 |
| 4426 | ND2 | ASN | A | 570 | 10.455 | 65.853 | 54.023 | 1.00 | 16.51 | 7 | 4468 | C   | ASN  | A | 575 | 7.578  | 73.682 | 39.820 | 1.00 | 12.18 | 6 |
| 4427 | N   | LEU | A | 571 | 7.108  | 68.381 | 53.486 | 1.00 | 14.82 | 7 | 4469 | C   | ASN  | A | 575 | 6.738  | 73.306 | 38.608 | 1.00 | 12.59 | 6 |

|      |     |           |       |        |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|-------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4468 | O   | ASN A 575 | 7.171 | 72.699 | 37.598 | 1.00 | 12.20 | 8 | 4510 | CB  | GLN A 581 | 8.751  | 75.601 | 27.465 | 1.00 | 11.27 | 6 |
| 4469 | CB  | ASN A 575 | 8.898 | 74.351 | 39.331 | 1.00 | 12.02 | 6 | 4511 | CG  | GLN A 581 | 8.407  | 75.301 | 28.975 | 1.00 | 10.49 | 6 |
| 4470 | CG  | ASN A 575 | 8.635 | 75.707 | 38.700 | 1.00 | 17.00 | 6 | 4512 | CD  | GLN A 581 | 7.920  | 76.579 | 29.654 | 1.00 | 12.45 | 6 |
| 4471 | OD1 | ASN A 575 | 7.562 | 76.292 | 38.872 | 1.00 | 14.54 | 8 | 4513 | OE1 | GLN A 581 | 8.545  | 77.588 | 29.921 | 1.00 | 13.44 | 8 |
| 4472 | ND2 | ASN A 575 | 9.608 | 76.223 | 37.934 | 1.00 | 13.02 | 7 | 4514 | NE2 | GLN A 581 | 6.582  | 76.528 | 30.002 | 1.00 | 11.11 | 7 |
| 4473 | N   | ILE A 576 | 5.400 | 73.515 | 38.739 | 1.00 | 10.95 | 7 | 4515 | N   | THR A 582 | 8.202  | 77.209 | 24.953 | 1.00 | 9.52  | 7 |
| 4474 | CA  | ILE A 576 | 4.506 | 73.221 | 37.604 | 1.00 | 10.36 | 6 | 4516 | CA  | THR A 582 | 8.978  | 77.646 | 23.772 | 1.00 | 10.13 | 6 |
| 4475 | C   | ILE A 576 | 4.485 | 74.374 | 36.602 | 1.00 | 12.05 | 6 | 4517 | C   | THR A 582 | 10.049 | 78.609 | 24.293 | 1.00 | 10.70 | 6 |
| 4476 | O   | ILE A 576 | 4.145 | 75.497 | 36.930 | 1.00 | 13.39 | 8 | 4518 | O   | THR A 582 | 9.921  | 79.235 | 25.313 | 1.00 | 12.73 | 8 |
| 4477 | CB  | ILE A 576 | 3.036 | 73.061 | 38.127 | 1.00 | 12.95 | 6 | 4519 | CB  | THR A 582 | 8.018  | 78.306 | 22.763 | 1.00 | 12.88 | 6 |
| 4478 | CG1 | ILE A 576 | 3.082 | 71.956 | 39.190 | 1.00 | 13.10 | 6 | 4520 | OG1 | THR A 582 | 8.736  | 78.798 | 21.599 | 1.00 | 12.92 | 8 |
| 4479 | CG2 | ILE A 576 | 2.079 | 72.677 | 36.966 | 1.00 | 14.18 | 6 | 4521 | CG2 | THR A 582 | 7.265  | 79.504 | 23.359 | 1.00 | 11.55 | 6 |
| 4480 | CD1 | ILE A 576 | 1.709 | 71.488 | 39.691 | 1.00 | 15.07 | 6 | 4522 | N   | SER A 583 | 11.166 | 78.712 | 23.507 | 1.00 | 11.67 | 7 |
| 4481 | N   | LEU A 577 | 4.883 | 74.054 | 35.368 | 1.00 | 10.51 | 7 | 4523 | CA  | SER A 583 | 12.321 | 79.527 | 23.931 | 1.00 | 12.58 | 6 |
| 4482 | CA  | LEU A 577 | 4.908 | 75.052 | 34.303 | 1.00 | 12.74 | 6 | 4524 | C   | SER A 583 | 12.300 | 80.783 | 23.061 | 1.00 | 11.58 | 6 |
| 4483 | C   | LEU A 577 | 3.480 | 75.308 | 33.772 | 1.00 | 11.80 | 6 | 4525 | O   | SER A 583 | 12.496 | 80.687 | 21.844 | 1.00 | 12.44 | 8 |
| 4484 | O   | LEU A 577 | 2.572 | 74.474 | 34.021 | 1.00 | 13.37 | 8 | 4526 | CB  | SER A 583 | 13.612 | 78.697 | 23.747 | 1.00 | 12.53 | 6 |
| 4485 | CB  | LEU A 577 | 5.757 | 74.463 | 33.137 | 1.00 | 11.48 | 6 | 4527 | OG  | SER A 583 | 14.755 | 79.449 | 24.240 | 1.00 | 14.73 | 8 |
| 4486 | CG  | LEU A 577 | 7.226 | 74.238 | 33.569 | 1.00 | 12.21 | 6 | 4528 | N   | VAL A 584 | 12.118 | 81.899 | 23.781 | 1.00 | 10.19 | 7 |
| 4487 | CD1 | LEU A 577 | 7.982 | 73.601 | 32.421 | 1.00 | 13.03 | 6 | 4529 | CA  | VAL A 584 | 11.741 | 83.141 | 23.016 | 1.00 | 9.76  | 6 |
| 4488 | CD2 | LEU A 577 | 7.897 | 75.576 | 33.989 | 1.00 | 13.85 | 6 | 4530 | C   | VAL A 584 | 12.721 | 84.268 | 23.298 | 1.00 | 11.27 | 6 |
| 4489 | N   | SER A 578 | 3.398 | 76.385 | 33.006 | 1.00 | 11.76 | 7 | 4531 | O   | VAL A 584 | 13.066 | 84.570 | 24.440 | 1.00 | 11.87 | 8 |
| 4490 | CA  | SER A 578 | 2.037 | 76.726 | 32.475 | 1.00 | 15.00 | 6 | 4532 | CB  | VAL A 584 | 10.358 | 83.645 | 23.506 | 1.00 | 12.33 | 6 |
| 4491 | C   | SER A 578 | 1.681 | 75.960 | 31.215 | 1.00 | 17.37 | 6 | 4533 | CG1 | VAL A 584 | 10.041 | 84.968 | 22.757 | 1.00 | 14.53 | 6 |
| 4492 | O   | SER A 578 | 0.553 | 76.134 | 30.685 | 1.00 | 17.93 | 8 | 4534 | CG2 | VAL A 584 | 9.279  | 82.604 | 23.220 | 1.00 | 12.71 | 6 |
| 4493 | CB  | SER A 578 | 2.081 | 78.230 | 32.132 | 1.00 | 13.25 | 6 | 4535 | N   | VAL A 585 | 13.307 | 84.868 | 22.244 | 1.00 | 10.77 | 7 |
| 4494 | OG  | SER A 578 | 2.321 | 78.967 | 33.305 | 1.00 | 14.45 | 8 | 4536 | CA  | VAL A 585 | 14.166 | 86.030 | 22.421 | 1.00 | 9.69  | 6 |
| 4495 | N   | GLY A 579 | 2.538 | 75.095 | 30.688 | 1.00 | 15.28 | 7 | 4537 | C   | VAL A 585 | 13.244 | 87.219 | 22.693 | 1.00 | 12.06 | 6 |
| 4496 | CA  | GLY A 579 | 2.266 | 74.270 | 29.497 | 1.00 | 14.88 | 6 | 4538 | O   | VAL A 585 | 12.450 | 87.576 | 21.803 | 1.00 | 14.60 | 8 |
| 4497 | C   | GLY A 579 | 3.627 | 74.010 | 28.818 | 1.00 | 13.39 | 6 | 4539 | CB  | VAL A 585 | 14.882 | 86.310 | 21.064 | 1.00 | 11.53 | 6 |
| 4498 | O   | GLY A 579 | 4.670 | 74.450 | 29.318 | 1.00 | 14.78 | 8 | 4540 | CG1 | VAL A 585 | 15.712 | 87.605 | 21.158 | 1.00 | 15.03 | 6 |
| 4499 | N   | THR A 580 | 3.518 | 73.227 | 27.740 | 1.00 | 11.35 | 7 | 4541 | CG2 | VAL A 585 | 15.750 | 85.111 | 20.717 | 1.00 | 14.67 | 6 |
| 4500 | CA  | THR A 580 | 4.803 | 72.961 | 27.005 | 1.00 | 13.16 | 6 | 4542 | N   | PHE A 586 | 13.361 | 87.762 | 23.908 | 1.00 | 12.32 | 7 |
| 4501 | C   | THR A 580 | 5.419 | 74.292 | 26.647 | 1.00 | 14.61 | 6 | 4543 | CA  | PHE A 586 | 12.622 | 88.986 | 24.243 | 1.00 | 12.19 | 6 |
| 4502 | O   | THR A 580 | 4.747 | 75.282 | 26.349 | 1.00 | 14.26 | 8 | 4544 | C   | PHE A 586 | 13.584 | 90.161 | 24.063 | 1.00 | 14.77 | 6 |
| 4503 | CB  | THR A 580 | 4.517 | 72.009 | 25.835 | 1.00 | 13.57 | 6 | 4545 | O   | PHE A 586 | 14.668 | 90.209 | 24.709 | 1.00 | 12.38 | 8 |
| 4504 | OG1 | THR A 580 | 5.753 | 71.676 | 25.176 | 1.00 | 16.06 | 8 | 4546 | CB  | PHE A 586 | 12.174 | 88.944 | 25.704 | 1.00 | 12.57 | 6 |
| 4505 | CG2 | THR A 580 | 3.688 | 72.715 | 24.732 | 1.00 | 20.75 | 6 | 4547 | CG  | PHE A 586 | 10.886 | 88.184 | 25.987 | 1.00 | 11.39 | 6 |
| 4506 | N   | GLN A 581 | 6.787 | 74.346 | 26.706 | 1.00 | 11.89 | 7 | 4548 | CD1 | PHE A 586 | 10.879 | 86.809 | 26.009 | 1.00 | 13.56 | 6 |
| 4507 | CA  | GLN A 581 | 7.454 | 75.658 | 26.609 | 1.00 | 10.06 | 6 | 4549 | CD2 | PHE A 586 | 9.694  | 88.868 | 26.231 | 1.00 | 13.70 | 6 |
| 4508 | C   | GLN A 581 | 8.012 | 75.905 | 25.148 | 1.00 | 10.19 | 6 | 4550 | CE1 | PHE A 586 | 9.758  | 86.060 | 26.284 | 1.00 | 13.86 | 6 |
| 4509 | O   | GLN A 581 | 8.163 | 75.020 | 24.338 | 1.00 | 12.94 | 8 | 4551 | CE2 | PHE A 586 | 8.543  | 88.102 | 26.520 | 1.00 | 12.32 | 6 |

|      |     |           |        |         |        |      |       |   |      |     |           |        |         |        |      |       |   |
|------|-----|-----------|--------|---------|--------|------|-------|---|------|-----|-----------|--------|---------|--------|------|-------|---|
| 4552 | CZ  | PHE A 586 | 8.577  | 86.707  | 26.558 | 1.00 | 11.70 | 6 | 4594 | N   | PRO A 593 | 18.778 | 105.367 | 29.550 | 1.00 | 21.02 | 7 |
| 4553 | N   | THR A 587 | 13.189 | 91.146  | 23.239 | 1.00 | 14.16 | 7 | 4595 | CA  | PRO A 593 | 20.204 | 105.252 | 29.779 | 1.00 | 20.83 | 6 |
| 4554 | CA  | THR A 587 | 14.016 | 92.324  | 23.066 | 1.00 | 12.96 | 6 | 4596 | C   | PRO A 593 | 20.494 | 104.537 | 31.094 | 1.00 | 20.17 | 6 |
| 4555 | C   | THR A 587 | 13.247 | 93.561  | 23.468 | 1.00 | 13.58 | 6 | 4597 | O   | PRO A 593 | 19.811 | 104.784 | 32.102 | 1.00 | 21.50 | 8 |
| 4556 | O   | THR A 587 | 12.072 | 93.651  | 23.058 | 1.00 | 15.22 | 8 | 4598 | CB  | PRO A 593 | 20.715 | 106.727 | 29.941 | 1.00 | 22.70 | 6 |
| 4557 | CB  | THR A 587 | 14.421 | 92.464  | 21.555 | 1.00 | 11.66 | 6 | 4599 | CG  | PRO A 593 | 19.643 | 107.491 | 29.165 | 1.00 | 24.71 | 6 |
| 4558 | OG1 | THR A 587 | 15.145 | 91.299  | 21.141 | 1.00 | 15.06 | 8 | 4600 | CD  | PRO A 593 | 18.337 | 106.774 | 29.432 | 1.00 | 23.44 | 6 |
| 4559 | CG2 | THR A 587 | 15.331 | 93.708  | 21.318 | 1.00 | 13.37 | 6 | 4601 | N   | THR A 594 | 21.530 | 103.723 | 31.165 | 1.00 | 19.91 | 7 |
| 4560 | N   | VAL A 588 | 13.829 | 94.487  | 24.195 | 1.00 | 14.03 | 7 | 4602 | CA  | THR A 594 | 21.909 | 103.060 | 32.402 | 1.00 | 21.78 | 6 |
| 4561 | CA  | VAL A 588 | 13.156 | 95.779  | 24.469 | 1.00 | 14.79 | 6 | 4603 | C   | THR A 594 | 23.380 | 103.366 | 32.686 | 1.00 | 23.13 | 6 |
| 4562 | C   | VAL A 588 | 14.079 | 96.867  | 23.912 | 1.00 | 14.40 | 6 | 4604 | O   | THR A 594 | 24.138 | 103.737 | 31.787 | 1.00 | 23.96 | 8 |
| 4563 | O   | VAL A 588 | 15.258 | 97.015  | 24.225 | 1.00 | 15.56 | 8 | 4605 | CB  | THR A 594 | 21.729 | 101.521 | 32.292 | 1.00 | 23.27 | 6 |
| 4564 | CB  | VAL A 588 | 12.863 | 95.933  | 25.971 | 1.00 | 14.24 | 6 | 4606 | OG1 | THR A 594 | 22.466 | 101.094 | 31.140 | 1.00 | 20.06 | 8 |
| 4565 | CG1 | VAL A 588 | 14.111 | 95.935  | 26.870 | 1.00 | 14.60 | 6 | 4607 | CG2 | THR A 594 | 20.245 | 101.183 | 32.157 | 1.00 | 21.33 | 6 |
| 4566 | CG2 | VAL A 588 | 12.079 | 97.255  | 26.232 | 1.00 | 13.38 | 6 | 4608 | N   | ASN A 595 | 23.764 | 103.210 | 33.928 | 1.00 | 23.96 | 7 |
| 4567 | N   | LYS A 589 | 13.478 | 97.570  | 22.915 | 1.00 | 15.39 | 7 | 4609 | CA  | ASN A 595 | 25.142 | 103.193 | 34.370 | 1.00 | 28.93 | 6 |
| 4568 | CA  | LYS A 589 | 14.212 | 98.670  | 22.258 | 1.00 | 16.20 | 6 | 4610 | C   | ASN A 595 | 25.614 | 101.791 | 34.716 | 1.00 | 31.88 | 6 |
| 4569 | C   | LYS A 589 | 14.180 | 100.009 | 22.953 | 1.00 | 18.01 | 6 | 4611 | O   | ASN A 595 | 24.847 | 100.849 | 34.915 | 1.00 | 22.74 | 8 |
| 4570 | O   | LYS A 589 | 13.230 | 100.355 | 23.652 | 1.00 | 15.39 | 8 | 4612 | CB  | ASN A 595 | 25.285 | 104.099 | 35.620 | 1.00 | 34.82 | 6 |
| 4571 | CB  | LYS A 589 | 13.597 | 98.820  | 20.860 | 1.00 | 16.23 | 6 | 4613 | CG  | ASN A 595 | 24.970 | 105.532 | 35.180 | 1.00 | 36.76 | 6 |
| 4572 | CG  | LYS A 589 | 13.908 | 97.588  | 20.008 | 1.00 | 17.01 | 6 | 4614 | OD1 | ASN A 595 | 24.047 | 106.190 | 35.647 | 1.00 | 42.57 | 8 |
| 4573 | CD  | LYS A 589 | 13.275 | 97.825  | 18.634 | 1.00 | 24.71 | 6 | 4615 | ND2 | ASN A 595 | 25.738 | 106.004 | 34.208 | 1.00 | 38.16 | 7 |
| 4574 | CE  | LYS A 589 | 13.494 | 96.582  | 17.792 | 1.00 | 37.49 | 6 | 4616 | N   | LEU A 596 | 26.939 | 101.654 | 34.839 | 1.00 | 34.83 | 7 |
| 4575 | NZ  | LYS A 589 | 13.368 | 96.852  | 16.321 | 1.00 | 51.36 | 7 | 4617 | CA  | LEU A 596 | 27.559 | 100.380 | 35.212 | 1.00 | 37.55 | 6 |
| 4576 | N   | LYS A 590 | 15.302 | 100.747 | 22.828 | 1.00 | 16.34 | 7 | 4618 | C   | LEU A 596 | 26.947 | 99.803  | 36.488 | 1.00 | 31.76 | 6 |
| 4577 | CA  | SER A 590 | 15.371 | 102.116 | 23.293 | 1.00 | 19.32 | 6 | 4619 | O   | LEU A 596 | 26.589 | 100.502 | 37.435 | 1.00 | 35.49 | 8 |
| 4578 | C   | SER A 590 | 15.006 | 102.295 | 24.746 | 1.00 | 19.68 | 6 | 4620 | CB  | LEU A 596 | 29.051 | 100.642 | 35.407 | 1.00 | 48.79 | 6 |
| 4579 | O   | SER A 590 | 14.185 | 103.146 | 25.151 | 1.00 | 17.24 | 8 | 4621 | CG  | LEU A 596 | 30.042 | 99.528  | 35.681 | 1.00 | 52.60 | 6 |
| 4580 | CB  | SER A 590 | 14.448 | 103.009 | 22.421 | 1.00 | 20.32 | 6 | 4622 | CD1 | LEU A 596 | 29.894 | 98.971  | 37.092 | 1.00 | 56.16 | 6 |
| 4581 | OG  | SER A 590 | 14.867 | 102.933 | 21.046 | 1.00 | 22.81 | 8 | 4623 | CD2 | LEU A 596 | 29.934 | 98.433  | 34.628 | 1.00 | 56.63 | 6 |
| 4582 | N   | ALA A 591 | 15.698 | 101.514 | 25.612 | 1.00 | 17.08 | 7 | 4624 | N   | GLY A 597 | 26.492 | 98.556  | 36.348 | 1.00 | 30.34 | 7 |
| 4583 | CA  | ALA A 591 | 15.458 | 101.617 | 27.048 | 1.00 | 16.02 | 6 | 4625 | CA  | GLY A 597 | 25.861 | 97.860  | 37.473 | 1.00 | 30.50 | 6 |
| 4584 | C   | ALA A 591 | 16.178 | 102.871 | 27.530 | 1.00 | 18.06 | 6 | 4626 | C   | GLY A 597 | 24.337 | 97.822  | 37.288 | 1.00 | 25.20 | 6 |
| 4585 | O   | ALA A 591 | 17.152 | 103.325 | 26.878 | 1.00 | 15.85 | 8 | 4627 | O   | GLY A 597 | 23.705 | 96.996  | 37.949 | 1.00 | 23.57 | 8 |
| 4586 | CB  | ALA A 591 | 16.045 | 100.326 | 27.695 | 1.00 | 15.17 | 6 | 4628 | N   | ASP A 598 | 23.780 | 98.803  | 36.544 | 1.00 | 21.92 | 7 |
| 4587 | N   | PRO A 592 | 15.872 | 103.303 | 28.730 | 1.00 | 18.28 | 7 | 4629 | CA  | ASP A 598 | 22.315 | 98.799  | 36.399 | 1.00 | 18.64 | 6 |
| 4588 | CA  | PRO A 592 | 16.493 | 104.529 | 29.298 | 1.00 | 18.18 | 6 | 4630 | C   | ASP A 598 | 21.982 | 97.666  | 35.429 | 1.00 | 21.53 | 6 |
| 4589 | C   | PRO A 592 | 17.967 | 104.319 | 29.512 | 1.00 | 22.69 | 6 | 4631 | O   | ASP A 598 | 22.702 | 97.563  | 34.399 | 1.00 | 20.69 | 8 |
| 4590 | O   | PRO A 592 | 18.463 | 103.180 | 29.693 | 1.00 | 19.12 | 8 | 4632 | CB  | ASP A 598 | 21.814 | 100.096 | 35.763 | 1.00 | 17.61 | 6 |
| 4591 | CB  | PRO A 592 | 15.762 | 104.797 | 30.621 | 1.00 | 19.23 | 6 | 4633 | CG  | ASP A 598 | 22.046 | 101.382 | 36.536 | 1.00 | 20.17 | 6 |
| 4592 | CG  | PRO A 592 | 14.433 | 104.085 | 30.387 | 1.00 | 23.18 | 6 | 4634 | OD1 | ASP A 598 | 22.364 | 101.347 | 37.751 | 1.00 | 19.25 | 8 |
| 4593 | CD  | PRO A 592 | 14.795 | 102.833 | 29.585 | 1.00 | 17.71 | 6 | 4635 | OD2 | ASP A 598 | 21.858 | 102.432 | 35.868 | 1.00 | 22.20 | 8 |



|      |     |           |        |        |        |      |       |   |      |               |        |        |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 4636 | N   | LYS A 599 | 20.861 | 96.919 | 35.612 | 1.00 | 18.66 | 7 | 4678 | OG1 THR A 603 | 7.971  | 90.241 | 36.987 | 1.00 | 14.53 | 8 |
| 4637 | CA  | LYS A 599 | 20.593 | 95.891 | 34.605 | 1.00 | 15.76 | 6 | 4679 | CG2 THR A 603 | 8.152  | 92.414 | 35.971 | 1.00 | 15.35 | 6 |
| 4638 | C   | LYS A 599 | 19.056 | 95.824 | 34.461 | 1.00 | 11.90 | 6 | 4680 | N GLY A 604   | 6.310  | 89.331 | 34.489 | 1.00 | 11.51 | 7 |
| 4639 | O   | LYS A 599 | 18.320 | 96.237 | 35.358 | 1.00 | 19.04 | 8 | 4681 | CA GLY A 604  | 4.995  | 89.274 | 33.787 | 1.00 | 11.82 | 6 |
| 4640 | CB  | LYS A 599 | 21.049 | 94.484 | 35.006 | 1.00 | 23.86 | 6 | 4682 | C GLY A 604   | 4.042  | 88.348 | 34.530 | 1.00 | 12.03 | 6 |
| 4641 | CG  | LYS A 599 | 22.597 | 94.419 | 35.031 | 1.00 | 25.32 | 6 | 4683 | O GLY A 604   | 4.358  | 87.909 | 35.636 | 1.00 | 13.68 | 8 |
| 4642 | CD  | LYS A 599 | 23.118 | 93.007 | 35.252 | 1.00 | 26.43 | 6 | 4684 | N ASN A 605   | 2.911  | 88.082 | 33.859 | 1.00 | 12.03 | 7 |
| 4643 | CE  | LYS A 599 | 24.656 | 93.063 | 35.120 | 1.00 | 32.43 | 6 | 4685 | CA ASN A 605  | 1.782  | 87.516 | 34.637 | 1.00 | 11.85 | 6 |
| 4644 | NZ  | LYS A 599 | 25.179 | 91.656 | 35.106 | 1.00 | 35.89 | 7 | 4686 | C ASN A 605   | 1.680  | 86.017 | 34.575 | 1.00 | 12.50 | 6 |
| 4645 | N   | ILE A 600 | 18.623 | 95.442 | 33.287 | 1.00 | 13.51 | 7 | 4687 | O ASN A 605   | 0.615  | 85.441 | 34.625 | 1.00 | 14.07 | 8 |
| 4646 | CA  | ILE A 600 | 17.178 | 95.336 | 33.021 | 1.00 | 12.20 | 6 | 4688 | CB ASN A 605  | 0.481  | 88.161 | 34.031 | 1.00 | 13.77 | 6 |
| 4647 | C   | ILE A 600 | 16.746 | 93.886 | 33.130 | 1.00 | 13.74 | 6 | 4689 | CG ASN A 605  | 0.265  | 87.610 | 32.629 | 1.00 | 17.19 | 6 |
| 4648 | O   | ILE A 600 | 17.476 | 92.927 | 32.799 | 1.00 | 14.24 | 8 | 4690 | OD1 ASN A 605 | 1.080  | 87.101 | 31.828 | 1.00 | 13.63 | 8 |
| 4649 | CB  | ILE A 600 | 16.938 | 95.829 | 31.554 | 1.00 | 13.87 | 6 | 4691 | ND2 ASN A 605 | -1.025 | 87.681 | 32.165 | 1.00 | 16.36 | 7 |
| 4650 | CG1 | ILE A 600 | 17.249 | 97.335 | 31.566 | 1.00 | 21.52 | 6 | 4692 | N ILE A 606   | 2.823  | 85.308 | 34.560 | 1.00 | 13.26 | 7 |
| 4651 | CG2 | ILE A 600 | 15.499 | 95.618 | 31.051 | 1.00 | 15.85 | 6 | 4693 | CA ILE A 606  | 2.836  | 83.860 | 34.628 | 1.00 | 11.73 | 6 |
| 4652 | CD1 | ILE A 600 | 16.798 | 98.104 | 30.313 | 1.00 | 23.52 | 6 | 4694 | C ILE A 606   | 4.099  | 83.493 | 35.448 | 1.00 | 13.02 | 6 |
| 4653 | N   | TYR A 601 | 15.545 | 93.745 | 33.676 | 1.00 | 13.09 | 7 | 4695 | O ILE A 606   | 5.005  | 84.349 | 35.511 | 1.00 | 13.34 | 8 |
| 4654 | CA  | TYR A 601 | 14.926 | 92.453 | 33.883 | 1.00 | 12.76 | 6 | 4696 | CB ILE A 606  | 2.995  | 83.184 | 33.259 | 1.00 | 11.81 | 6 |
| 4655 | C   | TYR A 601 | 13.531 | 92.475 | 33.288 | 1.00 | 13.27 | 6 | 4697 | CG1 ILE A 606 | 4.029  | 83.874 | 32.346 | 1.00 | 12.94 | 6 |
| 4656 | O   | TYR A 601 | 12.914 | 93.491 | 32.986 | 1.00 | 15.09 | 8 | 4698 | CG2 ILE A 606 | 1.625  | 83.138 | 32.550 | 1.00 | 15.56 | 6 |
| 4657 | CB  | TYR A 601 | 14.751 | 92.119 | 35.387 | 1.00 | 14.11 | 6 | 4699 | CD1 ILE A 606 | 4.300  | 82.981 | 31.113 | 1.00 | 15.13 | 6 |
| 4658 | CG  | TYR A 601 | 16.065 | 91.805 | 36.078 | 1.00 | 11.98 | 6 | 4700 | N PRO A 607   | 4.181  | 82.331 | 36.033 | 1.00 | 13.09 | 7 |
| 4659 | CD1 | TYR A 601 | 16.902 | 92.834 | 36.502 | 1.00 | 12.52 | 6 | 4701 | CA PRO A 607  | 5.294  | 81.982 | 36.937 | 1.00 | 12.68 | 6 |
| 4660 | CD2 | TYR A 601 | 16.473 | 90.490 | 36.242 | 1.00 | 12.95 | 6 | 4702 | C PRO A 607   | 6.616  | 81.880 | 36.189 | 1.00 | 10.98 | 6 |
| 4661 | CE1 | TYR A 601 | 18.138 | 92.544 | 37.097 | 1.00 | 13.54 | 6 | 4703 | O PRO A 607   | 4.895  | 80.647 | 37.607 | 1.00 | 14.73 | 8 |
| 4662 | CE2 | TYR A 601 | 17.673 | 90.213 | 36.888 | 1.00 | 14.26 | 6 | 4704 | CB PRO A 607  | 4.895  | 80.118 | 36.675 | 1.00 | 16.48 | 6 |
| 4663 | CZ  | TYR A 601 | 18.499 | 91.239 | 37.276 | 1.00 | 15.84 | 6 | 4705 | CG PRO A 607  | 3.818  | 80.118 | 36.675 | 1.00 | 16.43 | 6 |
| 4664 | OH  | TYR A 601 | 19.691 | 90.903 | 37.935 | 1.00 | 16.92 | 8 | 4706 | CD PRO A 607  | 3.081  | 81.335 | 36.098 | 1.00 | 16.43 | 6 |
| 4665 | N   | LEU A 602 | 12.986 | 91.285 | 33.068 | 1.00 | 11.99 | 7 | 4707 | N GLU A 608   | 6.531  | 81.525 | 34.880 | 1.00 | 11.74 | 7 |
| 4666 | CA  | LEU A 602 | 11.657 | 91.057 | 32.494 | 1.00 | 13.20 | 6 | 4708 | CA GLU A 608  | 7.747  | 81.559 | 34.031 | 1.00 | 10.58 | 6 |
| 4667 | C   | LEU A 602 | 10.762 | 90.434 | 33.580 | 1.00 | 14.26 | 6 | 4709 | C GLU A 608   | 8.382  | 82.958 | 33.994 | 1.00 | 13.60 | 6 |
| 4668 | O   | LEU A 602 | 11.148 | 89.522 | 34.284 | 1.00 | 13.06 | 8 | 4710 | O GLU A 608   | 9.606  | 83.060 | 33.731 | 1.00 | 11.79 | 8 |
| 4669 | CB  | LEU A 602 | 11.794 | 90.060 | 31.334 | 1.00 | 13.29 | 6 | 4711 | CB GLU A 608  | 7.437  | 81.056 | 32.616 | 1.00 | 11.09 | 6 |
| 4670 | CG  | LEU A 602 | 10.506 | 89.432 | 30.800 | 1.00 | 10.59 | 6 | 4712 | CG GLU A 608  | 7.145  | 79.550 | 32.522 | 1.00 | 10.94 | 6 |
| 4671 | CD1 | LEU A 602 | 9.579  | 90.481 | 30.155 | 1.00 | 14.08 | 6 | 4713 | CD GLU A 608  | 5.674  | 79.163 | 32.699 | 1.00 | 14.31 | 6 |
| 4672 | CD2 | LEU A 602 | 10.864 | 88.385 | 29.704 | 1.00 | 11.83 | 6 | 4714 | OE1 GLU A 608 | 4.875  | 79.973 | 33.221 | 1.00 | 12.87 | 8 |
| 4673 | N   | THR A 603 | 9.482  | 90.861 | 33.649 | 1.00 | 12.02 | 7 | 4715 | OE2 GLU A 608 | 5.344  | 78.040 | 32.280 | 1.00 | 13.22 | 8 |
| 4674 | CA  | THR A 603 | 8.570  | 90.233 | 34.635 | 1.00 | 12.81 | 6 | 4716 | N LEU A 609   | 7.571  | 83.999 | 34.112 | 1.00 | 11.31 | 7 |
| 4675 | C   | THR A 603 | 7.158  | 90.267 | 34.066 | 1.00 | 12.50 | 6 | 4717 | CA LEU A 609  | 8.093  | 85.359 | 34.095 | 1.00 | 11.00 | 6 |
| 4676 | O   | THR A 603 | 6.876  | 91.096 | 33.183 | 1.00 | 14.59 | 8 | 4718 | C LEU A 609   | 7.944  | 86.002 | 35.453 | 1.00 | 12.01 | 6 |
| 4677 | CB  | THR A 603 | 8.711  | 90.983 | 35.969 | 1.00 | 14.38 | 6 | 4719 | O LEU A 609   | 7.959  | 87.224 | 35.602 | 1.00 | 14.24 | 8 |



|      |     |           |        |        |        |      |       |   |      |     |           |        |         |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|---------|--------|------|-------|---|
| 4804 | CB  | ASN A 621 | 8.676  | 81.346 | 39.732 | 1.00 | 10.99 | 6 | 4846 | CG  | LEU A 627 | 16.549 | 91.433  | 28.919 | 1.00 | 13.68 | 6 |
| 4805 | CG  | ASN A 621 | 8.656  | 79.972 | 39.084 | 1.00 | 11.13 | 6 | 4847 | CD1 | LEU A 627 | 15.771 | 91.075  | 30.200 | 1.00 | 16.08 | 6 |
| 4806 | OD1 | ASN A 621 | 9.398  | 79.689 | 38.141 | 1.00 | 13.90 | 8 | 4848 | CD2 | LEU A 627 | 15.630 | 92.370  | 28.084 | 1.00 | 16.33 | 6 |
| 4807 | ND2 | ASN A 621 | 7.742  | 79.105 | 39.596 | 1.00 | 13.32 | 7 | 4849 | N   | LEU A 628 | 20.804 | 91.374  | 28.421 | 1.00 | 12.55 | 7 |
| 4808 | N   | ASN A 622 | 11.106 | 84.199 | 40.048 | 1.00 | 13.97 | 7 | 4850 | CA  | LEU A 628 | 22.139 | 91.805  | 27.919 | 1.00 | 12.76 | 6 |
| 4809 | CA  | ASN A 622 | 11.116 | 85.623 | 40.322 | 1.00 | 11.35 | 6 | 4851 | C   | LEU A 628 | 21.994 | 92.999  | 26.973 | 1.00 | 15.67 | 6 |
| 4810 | C   | ASN A 622 | 11.418 | 86.389 | 39.037 | 1.00 | 12.47 | 6 | 4852 | O   | LEU A 628 | 20.910 | 93.197  | 26.394 | 1.00 | 14.76 | 8 |
| 4811 | O   | ASN A 622 | 11.090 | 85.862 | 37.960 | 1.00 | 12.66 | 8 | 4853 | CB  | LEU A 628 | 22.746 | 90.663  | 27.111 | 1.00 | 14.06 | 6 |
| 4812 | CB  | ASN A 622 | 12.073 | 85.956 | 41.471 | 1.00 | 12.54 | 6 | 4854 | CG  | LEU A 628 | 22.848 | 89.332  | 27.886 | 1.00 | 14.72 | 6 |
| 4813 | CG  | ASN A 622 | 13.543 | 85.545 | 41.151 | 1.00 | 12.82 | 6 | 4855 | CD1 | LEU A 628 | 23.526 | 88.239  | 27.056 | 1.00 | 12.14 | 6 |
| 4814 | OD1 | ASN A 622 | 13.811 | 85.093 | 40.044 | 1.00 | 12.82 | 6 | 4856 | CD2 | LEU A 628 | 23.659 | 89.508  | 29.185 | 1.00 | 20.12 | 6 |
| 4815 | ND2 | ASN A 622 | 14.377 | 85.753 | 42.196 | 1.00 | 13.72 | 7 | 4857 | N   | ALA A 629 | 23.117 | 93.699  | 26.702 | 1.00 | 16.33 | 7 |
| 4816 | N   | ALA A 623 | 11.883 | 87.626 | 39.098 | 1.00 | 11.27 | 7 | 4858 | CA  | ALA A 629 | 22.871 | 94.875  | 25.787 | 1.00 | 16.83 | 6 |
| 4817 | CA  | ALA A 623 | 12.088 | 88.339 | 37.812 | 1.00 | 12.38 | 6 | 4859 | C   | ALA A 629 | 23.983 | 95.083  | 24.795 | 1.00 | 15.77 | 6 |
| 4818 | C   | ALA A 623 | 13.107 | 87.592 | 36.947 | 1.00 | 13.25 | 6 | 4860 | O   | ALA A 629 | 24.610 | 96.177  | 24.707 | 1.00 | 15.92 | 8 |
| 4819 | O   | ALA A 623 | 14.035 | 87.018 | 37.469 | 1.00 | 13.43 | 8 | 4861 | CB  | ALA A 629 | 22.674 | 96.098  | 26.674 | 1.00 | 19.56 | 6 |
| 4820 | CB  | ALA A 623 | 12.586 | 89.748 | 38.120 | 1.00 | 14.46 | 6 | 4862 | N   | PRO A 630 | 24.278 | 94.136  | 23.970 | 1.00 | 16.96 | 7 |
| 4821 | N   | GLN A 624 | 12.905 | 87.740 | 35.631 | 1.00 | 12.11 | 7 | 4863 | CA  | PRO A 630 | 25.237 | 94.281  | 22.873 | 1.00 | 19.28 | 6 |
| 4822 | CA  | GLN A 624 | 13.742 | 87.034 | 34.660 | 1.00 | 11.87 | 6 | 4864 | C   | PRO A 630 | 24.773 | 95.400  | 21.940 | 1.00 | 21.06 | 6 |
| 4823 | C   | GLN A 624 | 14.828 | 87.912 | 34.071 | 1.00 | 12.70 | 6 | 4865 | O   | PRO A 630 | 25.633 | 96.015  | 21.314 | 1.00 | 23.58 | 8 |
| 4824 | O   | GLN A 624 | 14.646 | 89.092 | 33.762 | 1.00 | 13.14 | 8 | 4866 | CB  | PRO A 630 | 25.314 | 92.944  | 22.123 | 1.00 | 17.59 | 6 |
| 4825 | CB  | GLN A 624 | 12.880 | 86.477 | 33.521 | 1.00 | 14.55 | 6 | 4867 | CG  | PRO A 630 | 23.928 | 92.367  | 22.442 | 1.00 | 18.42 | 6 |
| 4826 | CG  | GLN A 624 | 11.779 | 85.492 | 34.084 | 1.00 | 13.33 | 6 | 4868 | CD  | PRO A 630 | 23.644 | 92.807  | 23.877 | 1.00 | 18.05 | 6 |
| 4827 | CD  | GLN A 624 | 12.451 | 84.323 | 34.754 | 1.00 | 14.35 | 6 | 4869 | N   | ASN A 631 | 23.464 | 95.562  | 21.768 | 1.00 | 17.93 | 7 |
| 4828 | OE1 | GLN A 624 | 13.213 | 83.546 | 34.096 | 1.00 | 15.81 | 8 | 4870 | CA  | ASN A 631 | 22.935 | 96.635  | 20.926 | 1.00 | 17.58 | 6 |
| 4829 | NE2 | GLN A 624 | 12.268 | 84.078 | 36.040 | 1.00 | 14.08 | 7 | 4871 | C   | ASN A 631 | 22.382 | 97.779  | 21.748 | 1.00 | 17.45 | 6 |
| 4830 | N   | GLY A 625 | 15.989 | 87.264 | 33.941 | 1.00 | 12.93 | 7 | 4872 | O   | ASN A 631 | 21.359 | 98.370  | 21.354 | 1.00 | 18.41 | 8 |
| 4831 | CA  | GLY A 625 | 17.183 | 87.950 | 33.418 | 1.00 | 12.61 | 6 | 4873 | CB  | ASN A 631 | 21.902 | 96.082  | 19.950 | 1.00 | 18.61 | 6 |
| 4832 | C   | GLY A 625 | 18.392 | 87.917 | 34.310 | 1.00 | 12.24 | 6 | 4874 | CG  | ASN A 631 | 22.400 | 94.876  | 19.161 | 1.00 | 28.21 | 6 |
| 4833 | O   | GLY A 625 | 18.497 | 86.888 | 34.934 | 1.00 | 13.82 | 8 | 4875 | OD1 | ASN A 631 | 21.838 | 93.764  | 19.168 | 1.00 | 27.73 | 8 |
| 4834 | N   | PRO A 626 | 19.296 | 88.815 | 34.131 | 1.00 | 12.81 | 7 | 4876 | ND2 | ASN A 631 | 23.476 | 95.224  | 18.455 | 1.00 | 19.54 | 7 |
| 4835 | CA  | PRO A 626 | 19.237 | 90.097 | 33.510 | 1.00 | 15.64 | 6 | 4877 | N   | TYR A 632 | 22.980 | 98.110  | 22.883 | 1.00 | 16.27 | 7 |
| 4836 | C   | PRO A 626 | 19.288 | 89.998 | 32.003 | 1.00 | 15.42 | 6 | 4878 | CA  | TYR A 632 | 22.570 | 99.229  | 23.700 | 1.00 | 17.84 | 6 |
| 4837 | O   | PRO A 626 | 19.675 | 88.992 | 31.364 | 1.00 | 15.65 | 8 | 4879 | C   | TYR A 632 | 22.255 | 100.496 | 22.909 | 1.00 | 19.89 | 6 |
| 4838 | CB  | PRO A 626 | 20.374 | 91.012 | 34.019 | 1.00 | 15.71 | 6 | 4880 | O   | TYR A 632 | 23.030 | 100.672 | 21.982 | 1.00 | 19.89 | 8 |
| 4839 | CG  | PRO A 626 | 21.401 | 89.927 | 34.320 | 1.00 | 14.63 | 6 | 4881 | CB  | TYR A 632 | 23.749 | 99.537  | 24.643 | 1.00 | 18.23 | 6 |
| 4840 | CD  | PRO A 626 | 20.565 | 88.780 | 34.858 | 1.00 | 13.83 | 6 | 4882 | CG  | TYR A 632 | 23.520 | 100.604 | 25.654 | 1.00 | 20.78 | 6 |
| 4841 | N   | LEU A 627 | 18.725 | 91.061 | 31.332 | 1.00 | 13.98 | 7 | 4883 | CD1 | TYR A 632 | 22.919 | 100.369 | 26.875 | 1.00 | 20.07 | 6 |
| 4842 | CA  | LEU A 627 | 18.935 | 91.116 | 29.881 | 1.00 | 13.16 | 6 | 4884 | CD2 | TYR A 632 | 23.839 | 101.933 | 25.333 | 1.00 | 22.98 | 6 |
| 4843 | C   | LEU A 627 | 20.364 | 91.609 | 29.649 | 1.00 | 14.14 | 6 | 4885 | CE1 | TYR A 632 | 22.700 | 101.367 | 27.797 | 1.00 | 22.62 | 6 |
| 4844 | O   | LEU A 627 | 21.024 | 92.215 | 30.527 | 1.00 | 14.86 | 8 | 4886 | CE2 | TYR A 632 | 23.578 | 102.953 | 26.223 | 1.00 | 23.64 | 6 |
| 4845 | CB  | LEU A 627 | 17.906 | 92.080 | 29.214 | 1.00 | 13.73 | 6 | 4887 | CZ  | TYR A 632 | 23.051 | 102.671 | 27.457 | 1.00 | 27.32 | 6 |

|      |     |           |        |         |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|---------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4888 | OH  | TYR A 632 | 22.814 | 103.670 | 28.369 | 1.00 | 23.27 | 8 | 4930 | CA  | TYR A 637 | 17.759 | 87.841 | 26.425 | 1.00 | 12.35 | 6 |
| 4889 | N   | PRO A 633 | 21.113 | 101.067 | 23.157 | 1.00 | 19.06 | 7 | 4931 | C   | TYR A 637 | 16.714 | 86.848 | 25.989 | 1.00 | 12.24 | 6 |
| 4890 | CA  | PRO A 633 | 20.194 | 101.103 | 24.225 | 1.00 | 16.58 | 6 | 4932 | O   | TYR A 637 | 15.911 | 87.135 | 25.088 | 1.00 | 12.49 | 8 |
| 4891 | C   | PRO A 633 | 19.087 | 100.033 | 24.123 | 1.00 | 15.76 | 6 | 4933 | CB  | TYR A 637 | 18.183 | 87.770 | 27.903 | 1.00 | 12.77 | 6 |
| 4892 | O   | PRO A 633 | 18.188 | 100.153 | 24.954 | 1.00 | 16.24 | 8 | 4934 | CG  | TYR A 637 | 19.035 | 86.513 | 28.195 | 1.00 | 13.33 | 6 |
| 4893 | CB  | PRO A 633 | 19.474 | 102.498 | 24.311 | 1.00 | 19.94 | 6 | 4935 | CD1 | TYR A 637 | 20.253 | 86.244 | 27.548 | 1.00 | 12.60 | 6 |
| 4894 | CG  | PRO A 633 | 19.449 | 102.810 | 22.846 | 1.00 | 24.00 | 6 | 4936 | CD2 | TYR A 637 | 18.595 | 85.573 | 29.127 | 1.00 | 10.55 | 6 |
| 4895 | CD  | PRO A 633 | 20.772 | 102.271 | 22.369 | 1.00 | 24.76 | 6 | 4937 | CE1 | TYR A 637 | 21.022 | 85.134 | 27.792 | 1.00 | 11.85 | 6 |
| 4896 | N   | ASP A 634 | 19.272 | 99.094  | 23.169 | 1.00 | 16.18 | 7 | 4938 | CE2 | TYR A 637 | 19.321 | 84.424 | 29.387 | 1.00 | 12.60 | 6 |
| 4897 | CA  | ASP A 634 | 18.330 | 97.978  | 23.121 | 1.00 | 16.48 | 6 | 4939 | CZ  | TYR A 637 | 20.521 | 84.221 | 28.728 | 1.00 | 11.69 | 6 |
| 4898 | C   | ASP A 634 | 18.923 | 96.792  | 23.937 | 1.00 | 15.97 | 6 | 4940 | OH  | TYR A 637 | 21.255 | 83.073 | 29.016 | 1.00 | 11.85 | 8 |
| 4899 | O   | ASP A 634 | 20.153 | 96.671  | 24.058 | 1.00 | 16.27 | 8 | 4941 | N   | VAL A 638 | 16.857 | 85.565 | 26.379 | 1.00 | 12.66 | 7 |
| 4900 | CB  | ASP A 634 | 18.133 | 97.402  | 21.731 | 1.00 | 15.05 | 6 | 4942 | CA  | VAL A 638 | 16.033 | 84.508 | 25.827 | 1.00 | 10.90 | 6 |
| 4901 | CG  | ASP A 634 | 17.626 | 98.434  | 20.695 | 1.00 | 20.07 | 6 | 4943 | C   | VAL A 638 | 15.492 | 83.693 | 27.023 | 1.00 | 11.04 | 6 |
| 4902 | OD1 | ASP A 634 | 17.138 | 99.519  | 21.100 | 1.00 | 17.34 | 8 | 4944 | O   | VAL A 638 | 16.202 | 83.367 | 27.980 | 1.00 | 13.35 | 8 |
| 4903 | OD2 | ASP A 634 | 17.728 | 98.097  | 19.503 | 1.00 | 19.32 | 8 | 4945 | CB  | VAL A 638 | 16.830 | 83.496 | 24.987 | 1.00 | 12.00 | 6 |
| 4904 | N   | TRP A 635 | 18.009 | 96.147  | 24.656 | 1.00 | 14.45 | 7 | 4946 | CG1 | VAL A 638 | 15.922 | 82.650 | 24.118 | 1.00 | 12.74 | 6 |
| 4905 | CA  | TRP A 635 | 18.413 | 95.017  | 25.510 | 1.00 | 16.15 | 6 | 4947 | CG2 | VAL A 638 | 17.799 | 84.300 | 24.074 | 1.00 | 10.59 | 6 |
| 4906 | C   | TRP A 635 | 17.708 | 93.736  | 25.082 | 1.00 | 13.84 | 6 | 4948 | N   | PHE A 639 | 14.137 | 83.517 | 26.957 | 1.00 | 12.77 | 7 |
| 4907 | O   | TRP A 635 | 16.590 | 93.820  | 24.606 | 1.00 | 13.90 | 8 | 4949 | CA  | PHE A 639 | 13.441 | 82.960 | 28.082 | 1.00 | 9.34  | 6 |
| 4908 | CB  | TRP A 635 | 18.024 | 95.299  | 26.962 | 1.00 | 15.52 | 6 | 4950 | C   | PHE A 639 | 12.466 | 81.877 | 27.665 | 1.00 | 11.56 | 6 |
| 4909 | CG  | TRP A 635 | 18.818 | 96.421  | 27.587 | 1.00 | 14.07 | 6 | 4951 | O   | PHE A 639 | 11.814 | 81.982 | 26.632 | 1.00 | 12.26 | 8 |
| 4910 | CD1 | TRP A 635 | 18.737 | 97.739  | 27.178 | 1.00 | 14.13 | 6 | 4952 | CB  | PHE A 639 | 12.612 | 84.072 | 28.807 | 1.00 | 11.50 | 6 |
| 4911 | CD2 | TRP A 635 | 19.713 | 96.407  | 28.694 | 1.00 | 16.17 | 6 | 4953 | CG  | PHE A 639 | 13.498 | 85.209 | 29.322 | 1.00 | 12.29 | 6 |
| 4912 | NE1 | TRP A 635 | 19.561 | 98.533  | 27.989 | 1.00 | 15.61 | 7 | 4954 | CD1 | PHE A 639 | 14.294 | 85.042 | 30.446 | 1.00 | 11.38 | 6 |
| 4913 | CE2 | TRP A 635 | 20.179 | 97.706  | 28.908 | 1.00 | 17.77 | 6 | 4955 | CD2 | PHE A 639 | 13.567 | 86.380 | 28.563 | 1.00 | 13.67 | 6 |
| 4914 | CE3 | TRP A 635 | 20.179 | 95.350  | 29.511 | 1.00 | 18.51 | 6 | 4956 | CE1 | PHE A 639 | 15.176 | 86.094 | 30.829 | 1.00 | 12.05 | 6 |
| 4915 | CZ2 | TRP A 635 | 21.071 | 98.018  | 29.935 | 1.00 | 19.26 | 6 | 4957 | CE2 | PHE A 639 | 14.416 | 87.425 | 28.965 | 1.00 | 13.84 | 6 |
| 4916 | CZ3 | TRP A 635 | 21.100 | 95.671  | 30.515 | 1.00 | 23.17 | 6 | 4958 | CZ  | PHE A 639 | 15.196 | 87.301 | 30.113 | 1.00 | 13.28 | 6 |
| 4917 | CH2 | TRP A 635 | 21.514 | 96.992  | 30.735 | 1.00 | 20.92 | 6 | 4959 | N   | SER A 640 | 12.323 | 80.913 | 28.609 | 1.00 | 10.61 | 7 |
| 4918 | N   | PHE A 636 | 18.294 | 92.551  | 25.372 | 1.00 | 12.41 | 7 | 4960 | CA  | SER A 640 | 11.376 | 79.833 | 28.360 | 1.00 | 11.72 | 6 |
| 4919 | CA  | PHE A 636 | 17.562 | 91.335  | 24.947 | 1.00 | 11.57 | 6 | 4961 | C   | SER A 640 | 10.005 | 80.223 | 28.872 | 1.00 | 11.19 | 6 |
| 4920 | C   | PHE A 636 | 18.071 | 90.194  | 25.855 | 1.00 | 12.41 | 6 | 4962 | O   | SER A 640 | 9.878  | 80.649 | 30.026 | 1.00 | 12.90 | 8 |
| 4921 | O   | PHE A 636 | 19.204 | 90.239  | 26.345 | 1.00 | 13.24 | 8 | 4963 | CB  | SER A 640 | 11.915 | 78.568 | 29.132 | 1.00 | 12.23 | 6 |
| 4922 | CB  | PHE A 636 | 17.761 | 90.971  | 23.435 | 1.00 | 12.03 | 6 | 4964 | OG  | SER A 640 | 11.028 | 77.448 | 28.846 | 1.00 | 12.04 | 8 |
| 4923 | CG  | PHE A 636 | 19.030 | 90.118  | 23.261 | 1.00 | 12.15 | 6 | 4965 | N   | VAL A 641 | 9.007  | 80.190 | 27.975 | 1.00 | 8.82  | 7 |
| 4924 | CD1 | PHE A 636 | 20.287 | 90.667  | 23.292 | 1.00 | 17.38 | 6 | 4966 | CA  | VAL A 641 | 7.635  | 80.609 | 28.374 | 1.00 | 11.37 | 6 |
| 4925 | CD2 | PHE A 636 | 18.856 | 88.751  | 23.095 | 1.00 | 11.02 | 6 | 4967 | C   | VAL A 641 | 6.697  | 79.601 | 27.775 | 1.00 | 11.35 | 6 |
| 4926 | CE1 | PHE A 636 | 21.417 | 89.860  | 23.207 | 1.00 | 19.56 | 6 | 4968 | O   | VAL A 641 | 7.075  | 78.840 | 26.864 | 1.00 | 10.31 | 8 |
| 4927 | CE2 | PHE A 636 | 19.996 | 87.906  | 22.997 | 1.00 | 12.49 | 6 | 4969 | CB  | VAL A 641 | 7.286  | 82.019 | 27.760 | 1.00 | 11.50 | 6 |
| 4928 | CZ  | PHE A 636 | 21.250 | 88.466  | 23.034 | 1.00 | 17.21 | 6 | 4970 | CG1 | VAL A 641 | 8.061  | 83.038 | 28.624 | 1.00 | 13.20 | 6 |
| 4929 | N   | TYR A 637 | 17.229 | 89.170  | 25.966 | 1.00 | 12.09 | 7 | 4971 | CG2 | VAL A 641 | 7.607  | 82.115 | 26.241 | 1.00 | 10.82 | 6 |





|      |     |     |   |     |        |         |        |      |       |   |      |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5140 | NE1 | TRP | A | 662 | 7.781  | 98.218  | 39.608 | 1.00 | 21.46 | 7 | 5182 | CA  | HIS | A | 668 | 2.882  | 94.747 | 26.930 | 1.00 | 15.66 | 6 |
| 5141 | CE2 | TRP | A | 662 | 7.444  | 97.223  | 38.713 | 1.00 | 18.92 | 6 | 5183 | C   | HIS | A | 668 | 2.137  | 93.408 | 26.856 | 1.00 | 16.10 | 6 |
| 5142 | CE3 | TRP | A | 662 | 7.213  | 96.960  | 36.295 | 1.00 | 18.78 | 6 | 5184 | O   | HIS | A | 668 | 2.048  | 92.666 | 27.847 | 1.00 | 16.87 | 8 |
| 5143 | CZ2 | TRP | A | 662 | 6.994  | 95.923  | 38.966 | 1.00 | 16.39 | 6 | 5185 | CB  | HIS | A | 668 | 4.327  | 94.431 | 26.491 | 1.00 | 15.51 | 6 |
| 5144 | CZ3 | TRP | A | 662 | 6.798  | 95.661  | 36.537 | 1.00 | 18.67 | 6 | 5186 | CG  | HIS | A | 668 | 5.208  | 95.653 | 26.519 | 1.00 | 14.13 | 6 |
| 5145 | CH2 | TRP | A | 662 | 6.725  | 95.156  | 37.854 | 1.00 | 15.44 | 6 | 5187 | ND1 | HIS | A | 668 | 5.229  | 96.451 | 25.375 | 1.00 | 15.75 | 7 |
| 5146 | N   | GLU | A | 663 | 9.170  | 100.250 | 33.453 | 1.00 | 18.24 | 7 | 5188 | CD2 | HIS | A | 668 | 6.066  | 96.158 | 27.410 | 1.00 | 17.00 | 6 |
| 5147 | CA  | GLU | A | 663 | 8.551  | 100.857 | 32.292 | 1.00 | 17.79 | 6 | 5189 | CE1 | HIS | A | 668 | 6.108  | 97.464 | 25.592 | 1.00 | 14.21 | 6 |
| 5148 | C   | GLU | A | 663 | 7.240  | 101.517 | 32.740 | 1.00 | 17.95 | 6 | 5190 | NE2 | HIS | A | 668 | 6.581  | 97.305 | 26.830 | 1.00 | 15.51 | 7 |
| 5149 | O   | GLU | A | 663 | 6.519  | 100.973 | 33.574 | 1.00 | 18.49 | 8 | 5191 | N   | VAL | A | 669 | 1.434  | 93.208 | 25.734 | 1.00 | 15.02 | 7 |
| 5150 | CB  | GLU | A | 663 | 8.001  | 99.880  | 31.232 | 1.00 | 22.54 | 6 | 5192 | CA  | VAL | A | 669 | 0.684  | 91.987 | 25.490 | 1.00 | 16.94 | 6 |
| 5151 | CG  | GLU | A | 663 | 9.065  | 99.526  | 30.195 | 1.00 | 23.03 | 6 | 5193 | C   | VAL | A | 669 | 1.205  | 91.294 | 24.260 | 1.00 | 14.25 | 6 |
| 5152 | CD  | GLU | A | 663 | 8.380  | 98.560  | 29.223 | 1.00 | 19.52 | 6 | 5194 | O   | VAL | A | 669 | 1.414  | 91.936 | 23.206 | 1.00 | 17.08 | 8 |
| 5153 | OE1 | GLU | A | 663 | 8.159  | 97.397  | 29.619 | 1.00 | 17.12 | 8 | 5195 | CB  | VAL | A | 669 | -0.852 | 92.295 | 25.322 | 1.00 | 17.60 | 6 |
| 5154 | OE2 | GLU | A | 663 | 8.063  | 98.990  | 28.102 | 1.00 | 18.01 | 8 | 5196 | CG1 | VAL | A | 669 | -1.624 | 90.970 | 25.253 | 1.00 | 20.63 | 6 |
| 5155 | N   | ASN | A | 664 | 6.892  | 102.576 | 32.027 | 1.00 | 18.62 | 7 | 5197 | CG2 | VAL | A | 669 | -1.341 | 93.078 | 26.547 | 1.00 | 17.53 | 6 |
| 5156 | CA  | ASN | A | 664 | 5.604  | 103.189 | 32.365 | 1.00 | 18.27 | 6 | 5198 | N   | ALA | A | 670 | 1.450  | 89.971 | 24.287 | 1.00 | 14.50 | 7 |
| 5157 | C   | ASN | A | 664 | 4.522  | 102.581 | 31.484 | 1.00 | 20.85 | 6 | 5199 | CA  | ALA | A | 670 | 1.945  | 89.249 | 23.113 | 1.00 | 14.21 | 6 |
| 5158 | O   | ASN | A | 664 | 4.782  | 101.671 | 30.702 | 1.00 | 21.34 | 8 | 5200 | C   | ALA | A | 670 | 1.437  | 87.798 | 23.234 | 1.00 | 15.38 | 6 |
| 5159 | CB  | ASN | A | 664 | 5.790  | 104.696 | 32.115 | 1.00 | 22.20 | 6 | 5201 | O   | ALA | A | 670 | 1.216  | 87.262 | 24.323 | 1.00 | 15.04 | 8 |
| 5160 | CG  | ASN | A | 664 | 6.447  | 105.326 | 33.350 | 1.00 | 30.00 | 6 | 5202 | CB  | ALA | A | 670 | 3.481  | 89.251 | 23.005 | 1.00 | 14.71 | 6 |
| 5161 | OD1 | ASN | A | 664 | 6.281  | 104.932 | 34.519 | 1.00 | 35.11 | 8 | 5203 | N   | THR | A | 671 | 1.412  | 87.143 | 22.093 | 1.00 | 15.66 | 7 |
| 5162 | ND2 | ASN | A | 664 | 7.238  | 106.366 | 33.127 | 1.00 | 33.46 | 7 | 5204 | CA  | THR | A | 671 | 1.145  | 85.704 | 22.056 | 1.00 | 15.06 | 6 |
| 5163 | N   | GLY | A | 665 | 3.295  | 103.085 | 31.667 | 1.00 | 22.07 | 7 | 5205 | C   | THR | A | 671 | 2.463  | 85.017 | 21.737 | 1.00 | 15.13 | 6 |
| 5164 | CA  | GLY | A | 665 | 2.187  | 102.708 | 30.786 | 1.00 | 23.10 | 6 | 5206 | O   | THR | A | 671 | 3.141  | 85.293 | 20.734 | 1.00 | 16.78 | 8 |
| 5165 | C   | GLY | A | 665 | 1.557  | 101.363 | 31.102 | 1.00 | 21.34 | 6 | 5207 | CB  | THR | A | 671 | 0.004  | 85.374 | 21.082 | 1.00 | 24.32 | 6 |
| 5166 | O   | GLY | A | 665 | 1.827  | 100.710 | 32.119 | 1.00 | 22.70 | 8 | 5208 | OG1 | THR | A | 671 | -1.181 | 86.041 | 21.584 | 1.00 | 19.33 | 8 |
| 5167 | N   | SER | A | 666 | 0.832  | 100.839 | 30.093 | 1.00 | 18.43 | 7 | 5209 | CG2 | THR | A | 671 | -0.323 | 83.900 | 21.063 | 1.00 | 22.47 | 6 |
| 5168 | CA  | SER | A | 666 | 0.135  | 99.581  | 30.305 | 1.00 | 17.79 | 6 | 5210 | N   | THR | A | 672 | 2.794  | 83.967 | 22.533 | 1.00 | 13.36 | 7 |
| 5169 | C   | SER | A | 666 | 1.084  | 98.403  | 30.046 | 1.00 | 16.94 | 6 | 5211 | CA  | THR | A | 672 | 4.035  | 83.264 | 22.249 | 1.00 | 14.54 | 6 |
| 5170 | O   | SER | A | 666 | 2.005  | 98.503  | 29.261 | 1.00 | 16.68 | 8 | 5212 | C   | THR | A | 672 | 3.911  | 82.312 | 21.096 | 1.00 | 14.80 | 6 |
| 5171 | CB  | SER | A | 666 | -1.037 | 99.440  | 29.297 | 1.00 | 24.19 | 6 | 5213 | O   | THR | A | 672 | 2.831  | 81.798 | 20.772 | 1.00 | 13.92 | 8 |
| 5172 | OG  | SER | A | 666 | -1.959 | 100.498 | 29.645 | 1.00 | 24.86 | 8 | 5214 | CB  | THR | A | 672 | 4.475  | 82.464 | 23.491 | 1.00 | 15.06 | 6 |
| 5173 | N   | ASN | A | 667 | 0.642  | 97.227  | 30.470 | 1.00 | 14.27 | 7 | 5215 | OG1 | THR | A | 672 | 3.485  | 81.497 | 23.805 | 1.00 | 13.92 | 8 |
| 5174 | CA  | ASN | A | 667 | 1.491  | 96.058  | 30.168 | 1.00 | 16.75 | 6 | 5216 | CG2 | THR | A | 672 | 4.612  | 83.376 | 24.726 | 1.00 | 15.62 | 6 |
| 5175 | C   | ASN | A | 667 | 1.575  | 95.824  | 28.678 | 1.00 | 17.01 | 6 | 5217 | N   | PRO | A | 673 | 5.068  | 81.983 | 20.499 | 1.00 | 16.20 | 7 |
| 5176 | O   | ASN | A | 667 | 0.616  | 96.050  | 27.899 | 1.00 | 15.90 | 8 | 5218 | CA  | PRO | A | 673 | 5.116  | 81.063 | 19.381 | 1.00 | 21.02 | 6 |
| 5177 | CB  | ASN | A | 667 | 0.795  | 94.804  | 30.736 | 1.00 | 16.66 | 6 | 5219 | C   | PRO | A | 673 | 4.615  | 79.690 | 19.691 | 1.00 | 17.09 | 6 |
| 5178 | CG  | ASN | A | 667 | 0.703  | 94.817  | 32.248 | 1.00 | 19.33 | 6 | 5220 | O   | PRO | A | 673 | 4.691  | 79.290 | 20.893 | 1.00 | 16.99 | 8 |
| 5179 | OD1 | ASN | A | 667 | -0.178 | 94.105  | 32.855 | 1.00 | 20.96 | 8 | 5221 | CB  | PRO | A | 673 | 6.606  | 80.975 | 18.937 | 1.00 | 22.47 | 6 |
| 5180 | ND2 | ASN | A | 667 | 1.594  | 95.513  | 32.887 | 1.00 | 16.21 | 7 | 5222 | CG  | PRO | A | 673 | 7.309  | 81.859 | 19.872 | 1.00 | 22.50 | 6 |
| 5181 | N   | HIS | A | 668 | 2.720  | 95.243  | 28.272 | 1.00 | 13.63 | 7 | 5223 | CD  | PRO | A | 673 | 6.355  | 82.558 | 20.857 | 1.00 | 20.76 | 6 |

|      |     |           |        |        |        |      |       |   |      |     |           |        |         |        |      |       |   |
|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|---------|--------|------|-------|---|
| 5224 | N   | THR A 674 | 4.164  | 78.885 | 18.724 | 1.00 | 16.36 | 7 | 5266 | CD1 | ILE A 680 | 6.611  | 86.867  | 23.218 | 1.00 | 15.15 | 6 |
| 5225 | CA  | THR A 674 | 3.803  | 77.518 | 19.033 | 1.00 | 16.04 | 6 | 5267 | N   | THR A 681 | 9.363  | 91.378  | 20.334 | 1.00 | 13.57 | 7 |
| 5226 | C   | THR A 674 | 4.915  | 76.516 | 18.803 | 1.00 | 19.50 | 6 | 5268 | CA  | THR A 681 | 10.236 | 92.583  | 20.392 | 1.00 | 12.91 | 6 |
| 5227 | O   | THR A 674 | 4.834  | 75.399 | 19.293 | 1.00 | 25.45 | 8 | 5269 | C   | THR A 681 | 9.280  | 93.751  | 20.616 | 1.00 | 13.01 | 6 |
| 5228 | CB  | THR A 674 | 2.613  | 77.053 | 18.117 | 1.00 | 26.38 | 6 | 5270 | O   | THR A 681 | 8.253  | 93.845  | 19.929 | 1.00 | 18.59 | 8 |
| 5229 | OG1 | THR A 674 | 2.997  | 77.353 | 16.786 | 1.00 | 31.27 | 8 | 5271 | CB  | THR A 681 | 10.904 | 92.718  | 18.990 | 1.00 | 16.97 | 6 |
| 5230 | CG2 | THR A 674 | 1.409  | 77.936 | 18.521 | 1.00 | 27.63 | 6 | 5272 | OG1 | THR A 681 | 11.807 | 91.633  | 18.765 | 1.00 | 17.30 | 8 |
| 5231 | N   | GLY A 675 | 5.953  | 76.981 | 18.114 | 1.00 | 19.68 | 7 | 5273 | CG2 | THR A 681 | 11.642 | 94.052  | 18.964 | 1.00 | 19.53 | 6 |
| 5232 | CA  | GLY A 675 | 7.035  | 76.041 | 17.829 | 1.00 | 18.98 | 6 | 5274 | N   | VAL A 682 | 9.639  | 94.595  | 21.608 | 1.00 | 15.51 | 7 |
| 5233 | C   | GLY A 675 | 8.164  | 76.145 | 18.885 | 1.00 | 21.20 | 6 | 5275 | CA  | VAL A 682 | 8.758  | 95.732  | 21.946 | 1.00 | 15.78 | 6 |
| 5234 | O   | GLY A 675 | 7.915  | 76.654 | 19.953 | 1.00 | 18.10 | 8 | 5276 | C   | VAL A 682 | 9.635  | 96.952  | 22.186 | 1.00 | 17.87 | 6 |
| 5235 | N   | ALA A 676 | 9.349  | 75.612 | 18.560 | 1.00 | 14.92 | 7 | 5277 | O   | VAL A 682 | 10.838 | 96.797  | 22.256 | 1.00 | 15.49 | 8 |
| 5236 | CA  | ALA A 676 | 10.419 | 75.562 | 19.578 | 1.00 | 12.67 | 6 | 5278 | CB  | VAL A 682 | 7.874  | 95.472  | 23.195 | 1.00 | 16.15 | 6 |
| 5237 | C   | ALA A 676 | 10.845 | 76.968 | 19.974 | 1.00 | 13.87 | 6 | 5279 | CG1 | VAL A 682 | 6.968  | 94.243  | 23.002 | 1.00 | 16.76 | 6 |
| 5238 | O   | ALA A 676 | 11.505 | 77.096 | 21.031 | 1.00 | 12.93 | 8 | 5280 | CG2 | VAL A 682 | 8.730  | 95.365  | 24.469 | 1.00 | 16.17 | 6 |
| 5239 | CB  | ALA A 676 | 11.611 | 74.771 | 19.006 | 1.00 | 12.85 | 6 | 5281 | N   | THR A 683 | 9.082  | 98.162  | 22.306 | 1.00 | 15.89 | 7 |
| 5240 | N   | THR A 677 | 10.860 | 77.884 | 19.014 | 1.00 | 13.69 | 7 | 5282 | CA  | THR A 683 | 9.863  | 99.346  | 22.623 | 1.00 | 15.51 | 6 |
| 5241 | CA  | THR A 677 | 11.444 | 79.189 | 19.324 | 1.00 | 11.81 | 6 | 5283 | C   | THR A 683 | 9.529  | 99.798  | 24.046 | 1.00 | 16.36 | 6 |
| 5242 | C   | THR A 677 | 10.615 | 80.296 | 18.686 | 1.00 | 13.20 | 6 | 5284 | O   | THR A 683 | 8.371  | 99.703  | 24.462 | 1.00 | 17.59 | 8 |
| 5243 | O   | THR A 677 | 9.743  | 80.066 | 17.834 | 1.00 | 14.64 | 8 | 5285 | CB  | THR A 683 | 9.481  | 100.473 | 21.614 | 1.00 | 22.31 | 6 |
| 5244 | CB  | THR A 677 | 12.847 | 79.366 | 18.681 | 1.00 | 14.32 | 6 | 5286 | OG1 | THR A 683 | 9.916  | 100.019 | 20.328 | 1.00 | 21.22 | 8 |
| 5245 | OG1 | THR A 677 | 12.712 | 79.294 | 17.249 | 1.00 | 16.35 | 8 | 5287 | CG2 | THR A 683 | 10.245 | 101.759 | 21.921 | 1.00 | 19.31 | 6 |
| 5246 | CG2 | THR A 677 | 13.851 | 78.287 | 19.079 | 1.00 | 14.03 | 6 | 5288 | N   | TRP A 684 | 10.586 | 100.168 | 24.759 | 1.00 | 14.24 | 7 |
| 5247 | N   | GLY A 678 | 10.949 | 81.490 | 19.141 | 1.00 | 14.25 | 7 | 5289 | CA  | TRP A 684 | 10.411 | 100.587 | 26.154 | 1.00 | 14.76 | 6 |
| 5248 | CA  | GLY A 678 | 10.413 | 82.685 | 18.437 | 1.00 | 13.38 | 6 | 5290 | C   | TRP A 684 | 9.369  | 101.706 | 26.222 | 1.00 | 17.75 | 6 |
| 5249 | C   | GLY A 678 | 10.969 | 83.958 | 19.066 | 1.00 | 13.68 | 6 | 5291 | O   | TRP A 684 | 9.556  | 102.695 | 25.469 | 1.00 | 18.74 | 8 |
| 5250 | O   | GLY A 678 | 11.857 | 83.956 | 19.907 | 1.00 | 13.62 | 8 | 5292 | CB  | TRP A 684 | 11.745 | 101.086 | 26.705 | 1.00 | 14.95 | 6 |
| 5251 | N   | ASN A 679 | 10.374 | 85.094 | 18.654 | 1.00 | 13.18 | 7 | 5293 | CG  | TRP A 684 | 11.696 | 101.465 | 28.146 | 1.00 | 14.49 | 6 |
| 5252 | CA  | ASN A 679 | 10.858 | 86.398 | 19.082 | 1.00 | 11.86 | 6 | 5294 | CD1 | TRP A 684 | 11.284 | 102.666 | 28.672 | 1.00 | 15.39 | 6 |
| 5253 | C   | ASN A 679 | 9.685  | 87.318 | 19.466 | 1.00 | 14.28 | 6 | 5295 | CD2 | TRP A 684 | 12.163 | 100.683 | 29.271 | 1.00 | 17.84 | 6 |
| 5254 | O   | ASN A 679 | 8.718  | 87.315 | 18.699 | 1.00 | 15.54 | 8 | 5296 | NE1 | TRP A 684 | 11.376 | 102.649 | 30.052 | 1.00 | 16.11 | 7 |
| 5255 | CB  | ASN A 679 | 11.485 | 87.180 | 17.892 | 1.00 | 16.45 | 6 | 5297 | CE2 | TRP A 684 | 11.921 | 101.440 | 30.423 | 1.00 | 20.66 | 6 |
| 5256 | CG  | ASN A 679 | 12.952 | 86.818 | 17.758 | 1.00 | 25.76 | 6 | 5298 | CE3 | TRP A 684 | 12.764 | 99.422  | 29.399 | 1.00 | 18.28 | 6 |
| 5257 | OD1 | ASN A 679 | 13.201 | 85.708 | 17.294 | 1.00 | 24.19 | 8 | 5299 | CZ2 | TRP A 684 | 12.245 | 101.024 | 31.726 | 1.00 | 22.23 | 6 |
| 5258 | ND2 | ASN A 679 | 13.881 | 87.684 | 18.146 | 1.00 | 26.44 | 7 | 5300 | CZ3 | TRP A 684 | 13.074 | 98.959  | 30.709 | 1.00 | 17.05 | 6 |
| 5259 | N   | ILE A 680 | 9.882  | 88.063 | 20.521 | 1.00 | 13.28 | 7 | 5301 | CH2 | TRP A 684 | 12.791 | 99.766  | 31.796 | 1.00 | 17.97 | 6 |
| 5260 | CA  | ILE A 680 | 8.909  | 89.088 | 20.948 | 1.00 | 14.10 | 6 | 5302 | N   | GLN A 685 | 8.396  | 101.650 | 27.102 | 1.00 | 17.70 | 7 |
| 5261 | C   | ILE A 680 | 9.758  | 90.331 | 21.083 | 1.00 | 16.54 | 6 | 5303 | CA  | GLN A 685 | 7.399  | 102.716 | 27.315 | 1.00 | 18.97 | 6 |
| 5262 | O   | ILE A 680 | 10.673 | 90.366 | 21.944 | 1.00 | 14.10 | 8 | 5304 | C   | GLN A 685 | 7.850  | 103.719 | 28.333 | 1.00 | 19.08 | 6 |
| 5263 | CB  | ILE A 680 | 8.224  | 88.676 | 22.277 | 1.00 | 13.96 | 6 | 5305 | O   | GLN A 685 | 8.067  | 103.430 | 29.512 | 1.00 | 19.01 | 8 |
| 5264 | CG1 | ILE A 680 | 7.245  | 87.519 | 21.978 | 1.00 | 16.92 | 6 | 5306 | CB  | GLN A 685 | 6.071  | 102.025 | 27.745 | 1.00 | 15.69 | 6 |
| 5265 | CG2 | ILE A 680 | 7.442  | 89.919 | 22.790 | 1.00 | 17.42 | 6 | 5307 | CG  | GLN A 685 | 5.536  | 101.157 | 26.596 | 1.00 | 17.89 | 6 |



|      |     |           |        |         |        |      |       |   |      |     |           |        |        |        |      |       |   |
|------|-----|-----------|--------|---------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 5308 | CD  | GLN A 685 | 4.352  | 100.283 | 26.995 | 1.00 | 18.78 | 6 | 5350 | C36 | HEX A 690 | 37.084 | 73.167 | 28.829 | 1.00 | 13.71 | 6 |
| 5309 | OE1 | GLN A 685 | 3.797  | 99.604  | 26.110 | 1.00 | 20.58 | 8 | 5351 | C41 | HEX A 690 | 33.322 | 71.601 | 28.292 | 1.00 | 9.18  | 6 |
| 5310 | NE2 | GLN A 685 | 3.960  | 100.246 | 28.267 | 1.00 | 17.75 | 7 | 5352 | N41 | HEX A 690 | 34.214 | 72.300 | 29.267 | 1.00 | 10.73 | 7 |
| 5311 | N   | ASN A 686 | 8.037  | 105.011 | 27.906 | 1.00 | 21.27 | 7 | 5353 | C42 | HEX A 690 | 33.682 | 70.074 | 28.156 | 1.00 | 11.48 | 6 |
| 5312 | CA  | ASN A 686 | 8.547  | 106.008 | 28.836 | 1.00 | 20.38 | 6 | 5354 | O42 | HEX A 690 | 33.732 | 69.433 | 29.448 | 1.00 | 10.30 | 8 |
| 5313 | C   | ASN A 686 | 7.489  | 106.854 | 29.654 | 1.00 | 22.87 | 6 | 5355 | C43 | HEX A 690 | 35.023 | 69.963 | 27.455 | 1.00 | 10.39 | 6 |
| 5314 | O   | ASN A 686 | 6.387  | 106.692 | 29.016 | 1.00 | 22.87 | 8 | 5356 | O43 | HEX A 690 | 35.686 | 68.699 | 27.591 | 1.00 | 11.44 | 8 |
| 5315 | CB  | ASN A 686 | 9.300  | 107.060 | 27.975 | 1.00 | 24.12 | 6 | 5357 | C44 | HEX A 690 | 34.791 | 70.257 | 25.986 | 1.00 | 11.02 | 6 |
| 5316 | CG  | ASN A 686 | 10.434 | 106.404 | 27.176 | 1.00 | 23.38 | 6 | 5358 | C45 | HEX A 690 | 33.925 | 71.520 | 25.899 | 1.00 | 10.58 | 6 |
| 5317 | OD1 | ASN A 686 | 11.360 | 105.896 | 27.821 | 1.00 | 22.76 | 8 | 5359 | C40 | HEX A 690 | 33.262 | 72.097 | 26.944 | 1.00 | 9.08  | 6 |
| 5318 | ND2 | ASN A 686 | 10.376 | 106.412 | 25.832 | 1.00 | 25.47 | 7 | 5360 | C46 | HEX A 690 | 33.519 | 71.887 | 24.466 | 1.00 | 12.28 | 6 |
| 5319 | C11 | HEX A 690 | 38.644 | 78.012  | 38.228 | 1.00 | 27.46 | 6 | 5361 | O46 | HEX A 690 | 32.492 | 71.022 | 24.020 | 1.00 | 12.58 | 8 |
| 5320 | O11 | HEX A 690 | 39.147 | 78.243  | 39.503 | 1.00 | 37.24 | 8 | 5362 | C51 | HEX A 690 | 36.288 | 69.864 | 24.116 | 1.00 | 10.88 | 6 |
| 5321 | C12 | HEX A 690 | 37.596 | 79.172  | 38.058 | 1.00 | 23.95 | 6 | 5363 | O51 | HEX A 690 | 36.061 | 70.541 | 25.327 | 1.00 | 12.10 | 8 |
| 5322 | O12 | HEX A 690 | 36.681 | 78.887  | 39.109 | 1.00 | 20.96 | 8 | 5364 | C52 | HEX A 690 | 37.495 | 68.906 | 24.274 | 1.00 | 11.69 | 6 |
| 5323 | C13 | HEX A 690 | 36.915 | 78.887  | 36.685 | 1.00 | 17.64 | 6 | 5365 | O52 | HEX A 690 | 37.227 | 67.917 | 25.285 | 1.00 | 12.57 | 8 |
| 5324 | O13 | HEX A 690 | 35.915 | 79.908  | 36.442 | 1.00 | 18.04 | 8 | 5366 | C53 | HEX A 690 | 38.717 | 69.698 | 24.774 | 1.00 | 10.51 | 6 |
| 5325 | C14 | HEX A 690 | 38.048 | 79.023  | 35.670 | 1.00 | 17.74 | 6 | 5367 | O53 | HEX A 690 | 39.832 | 68.756 | 24.609 | 1.00 | 11.97 | 8 |
| 5326 | C15 | HEX A 690 | 39.141 | 77.967  | 35.956 | 1.00 | 19.52 | 6 | 5368 | C54 | HEX A 690 | 39.025 | 70.807 | 23.714 | 1.00 | 12.82 | 6 |
| 5327 | O15 | HEX A 690 | 39.679 | 78.312  | 37.276 | 1.00 | 26.20 | 8 | 5369 | C55 | HEX A 690 | 37.748 | 71.660 | 23.566 | 1.00 | 12.56 | 6 |
| 5328 | C16 | HEX A 690 | 40.338 | 77.919  | 35.016 | 1.00 | 23.71 | 6 | 5370 | O55 | HEX A 690 | 36.680 | 70.820 | 23.133 | 1.00 | 11.57 | 8 |
| 5329 | O16 | HEX A 690 | 40.867 | 79.240  | 34.817 | 1.00 | 28.38 | 8 | 5371 | C56 | HEX A 690 | 37.890 | 72.687 | 22.436 | 1.00 | 12.61 | 6 |
| 5330 | C21 | HEX A 690 | 37.609 | 79.324  | 33.250 | 1.00 | 19.03 | 6 | 5372 | O56 | HEX A 690 | 38.082 | 72.074 | 21.134 | 1.00 | 19.74 | 8 |
| 5331 | O21 | HEX A 690 | 37.414 | 78.562  | 34.414 | 1.00 | 18.39 | 8 | 5373 | C61 | HEX A 690 | 40.720 | 72.590 | 24.188 | 1.00 | 22.95 | 6 |
| 5332 | C22 | HEX A 690 | 36.237 | 79.756  | 32.692 | 1.00 | 18.97 | 6 | 5374 | O61 | HEX A 690 | 39.890 | 71.572 | 24.637 | 1.00 | 20.26 | 8 |
| 5333 | O22 | HEX A 690 | 35.419 | 80.404  | 33.669 | 1.00 | 17.96 | 8 | 5375 | C62 | HEX A 690 | 42.050 | 72.500 | 24.991 | 1.00 | 23.13 | 6 |
| 5334 | C23 | HEX A 690 | 35.514 | 78.516  | 32.153 | 1.00 | 16.72 | 6 | 5376 | O62 | HEX A 690 | 42.582 | 71.189 | 24.918 | 1.00 | 23.06 | 8 |
| 5335 | O23 | HEX A 690 | 34.355 | 79.014  | 31.406 | 1.00 | 16.31 | 8 | 5377 | C63 | HEX A 690 | 41.937 | 73.006 | 26.411 | 1.00 | 24.03 | 6 |
| 5336 | C24 | HEX A 690 | 36.415 | 77.760  | 31.174 | 1.00 | 12.77 | 6 | 5378 | O63 | HEX A 690 | 43.280 | 72.994 | 26.932 | 1.00 | 28.78 | 8 |
| 5337 | C25 | HEX A 690 | 37.690 | 77.301  | 31.955 | 1.00 | 17.32 | 6 | 5379 | C64 | HEX A 690 | 41.310 | 74.405 | 26.428 | 1.00 | 25.79 | 6 |
| 5338 | O25 | HEX A 690 | 38.321 | 78.596  | 32.286 | 1.00 | 20.72 | 8 | 5380 | O64 | HEX A 690 | 41.035 | 74.789 | 27.809 | 1.00 | 29.96 | 8 |
| 5339 | C26 | HEX A 690 | 38.704 | 76.681  | 30.979 | 1.00 | 18.94 | 6 | 5381 | C65 | HEX A 690 | 39.918 | 74.255 | 25.759 | 1.00 | 22.19 | 6 |
| 5340 | O26 | HEX A 690 | 39.852 | 76.182  | 31.780 | 1.00 | 21.07 | 8 | 5382 | O65 | HEX A 690 | 40.146 | 73.866 | 24.404 | 1.00 | 22.47 | 8 |
| 5341 | C31 | HEX A 690 | 35.507 | 76.403  | 29.409 | 1.00 | 11.28 | 6 | 5383 | C66 | HEX A 690 | 39.177 | 75.555 | 25.611 | 1.00 | 26.12 | 6 |
| 5342 | O31 | HEX A 690 | 35.723 | 76.501  | 30.811 | 1.00 | 12.85 | 8 | 5384 | O66 | HEX A 690 | 39.936 | 76.644 | 25.149 | 1.00 | 24.41 | 8 |
| 5343 | C32 | HEX A 690 | 34.026 | 76.118  | 29.118 | 1.00 | 13.04 | 6 | 5385 | C11 | MAL A 691 | 38.534 | 71.299 | 69.464 | 1.00 | 19.75 | 6 |
| 5344 | O32 | HEX A 690 | 33.259 | 77.030  | 29.933 | 1.00 | 14.06 | 8 | 5386 | O11 | MAL A 691 | 38.776 | 72.581 | 69.883 | 1.00 | 20.21 | 8 |
| 5345 | C33 | HEX A 690 | 33.654 | 74.698  | 29.626 | 1.00 | 13.59 | 6 | 5387 | C12 | MAL A 691 | 37.973 | 71.384 | 68.024 | 1.00 | 17.66 | 6 |
| 5346 | O33 | HEX A 690 | 32.285 | 74.486  | 29.158 | 1.00 | 12.48 | 8 | 5388 | O12 | MAL A 691 | 38.798 | 72.262 | 67.225 | 1.00 | 18.71 | 8 |
| 5347 | C34 | HEX A 690 | 34.578 | 73.670  | 28.936 | 1.00 | 11.83 | 6 | 5389 | C13 | MAL A 691 | 36.555 | 71.949 | 68.006 | 1.00 | 16.03 | 6 |
| 5348 | O35 | HEX A 690 | 36.004 | 74.036  | 29.487 | 1.00 | 14.01 | 6 | 5390 | O13 | MAL A 691 | 35.969 | 71.754 | 66.689 | 1.00 | 17.47 | 8 |
| 5349 | O35 | HEX A 690 | 36.301 | 75.341  | 28.930 | 1.00 | 12.70 | 8 | 5391 | C14 | MAL A 691 | 35.642 | 71.104 | 68.925 | 1.00 | 15.64 | 6 |

THE UNIVERSITY OF THE SOUTH PACIFIC  
SCHOOL OF DISTANCE EDUCATION  
SUVA, FIJI

|      |     |     |   |     |        |        |        |      |       |    |      |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 5392 | C15 | MAL | A | 691 | 36.269 | 71.291 | 70.364 | 1.00 | 14.01 | 6  | 5472 | OWO | WAT | V | 19 | 26.088 | 62.658 | 22.854 | 1.00 | 11.54 | 8 |
| 5393 | O15 | MAL | A | 691 | 37.561 | 70.667 | 70.312 | 1.00 | 16.48 | 8  | 5473 | OWO | WAT | V | 20 | 37.981 | 63.919 | 14.127 | 1.00 | 11.77 | 8 |
| 5394 | C16 | MAL | A | 691 | 35.519 | 70.221 | 71.238 | 1.00 | 19.77 | 6  | 5474 | OWO | WAT | V | 21 | 34.932 | 60.656 | 13.769 | 1.00 | 11.70 | 8 |
| 5395 | O16 | MAL | A | 691 | 36.004 | 70.431 | 72.581 | 1.00 | 18.54 | 8  | 5475 | OWO | WAT | V | 22 | 41.499 | 60.656 | 38.722 | 1.00 | 11.54 | 8 |
| 5396 | C21 | MAL | A | 691 | 33.285 | 70.813 | 68.523 | 1.00 | 18.83 | 6  | 5476 | OWO | WAT | V | 23 | 40.945 | 66.711 | 20.205 | 1.00 | 11.65 | 8 |
| 5397 | O21 | MAL | A | 691 | 34.336 | 71.683 | 68.968 | 1.00 | 17.92 | 8  | 5477 | OWO | WAT | V | 24 | 8.905  | 64.107 | 34.370 | 1.00 | 11.68 | 8 |
| 5398 | C22 | MAL | A | 691 | 32.403 | 71.638 | 67.561 | 1.00 | 17.24 | 6  | 5478 | OWO | WAT | V | 25 | 19.426 | 72.356 | 40.893 | 1.00 | 11.74 | 8 |
| 5399 | O22 | MAL | A | 691 | 33.177 | 72.083 | 66.433 | 1.00 | 17.89 | 8  | 5479 | OWO | WAT | V | 26 | 20.321 | 82.331 | 35.376 | 1.00 | 11.77 | 8 |
| 5400 | C23 | MAL | A | 691 | 31.765 | 72.820 | 68.304 | 1.00 | 18.41 | 6  | 5480 | OWO | WAT | V | 27 | 14.993 | 64.250 | 37.502 | 1.00 | 11.91 | 8 |
| 5401 | O23 | MAL | A | 691 | 30.812 | 73.419 | 67.431 | 1.00 | 18.30 | 8  | 5481 | OWO | WAT | V | 28 | 31.504 | 68.673 | 10.842 | 1.00 | 12.08 | 8 |
| 5402 | C24 | MAL | A | 691 | 30.951 | 72.194 | 69.478 | 1.00 | 18.57 | 6  | 5482 | OWO | WAT | V | 29 | 37.606 | 61.402 | 40.167 | 1.00 | 11.91 | 8 |
| 5403 | O24 | MAL | A | 691 | 30.444 | 73.291 | 70.263 | 1.00 | 19.15 | 8  | 5483 | OWO | WAT | V | 30 | 16.372 | 70.863 | 38.933 | 1.00 | 11.99 | 8 |
| 5404 | C25 | MAL | A | 691 | 31.923 | 71.424 | 70.383 | 1.00 | 19.32 | 6  | 5484 | OWO | WAT | V | 31 | 7.950  | 69.079 | 31.258 | 1.00 | 12.08 | 8 |
| 5405 | O25 | MAL | A | 691 | 32.521 | 70.374 | 69.608 | 1.00 | 18.98 | 8  | 5485 | OWO | WAT | V | 32 | 19.528 | 73.999 | 43.164 | 1.00 | 12.10 | 8 |
| 5406 | C26 | MAL | A | 691 | 31.067 | 70.708 | 71.468 | 1.00 | 15.38 | 6  | 5486 | OWO | WAT | V | 33 | 16.210 | 66.954 | 39.606 | 1.00 | 12.02 | 8 |
| 5407 | O26 | MAL | A | 691 | 31.944 | 70.075 | 72.412 | 1.00 | 18.74 | 8  | 5487 | OWO | WAT | V | 34 | 32.679 | 63.267 | 29.330 | 1.00 | 12.26 | 8 |
| 5411 | S   | SUL | A | 695 | 11.120 | 52.018 | 55.465 | 1.00 | 30.54 | 16 | 5488 | OWO | WAT | V | 35 | 13.649 | 74.479 | 39.683 | 1.00 | 12.21 | 8 |
| 5412 | O1  | SUL | A | 695 | 11.470 | 52.936 | 56.533 | 1.00 | 30.07 | 8  | 5489 | OWO | WAT | V | 36 | 16.357 | 79.631 | 22.013 | 1.00 | 12.26 | 8 |
| 5413 | O2  | SUL | A | 695 | 10.034 | 52.528 | 54.544 | 1.00 | 27.19 | 8  | 5490 | OWO | WAT | V | 37 | 21.471 | 63.888 | 43.225 | 1.00 | 12.25 | 8 |
| 5414 | O3  | SUL | A | 695 | 12.310 | 51.631 | 54.662 | 1.00 | 34.25 | 8  | 5491 | OWO | WAT | V | 38 | 42.464 | 66.587 | 23.881 | 1.00 | 12.49 | 8 |
| 5415 | O4  | SUL | A | 695 | 10.566 | 50.749 | 56.089 | 1.00 | 33.96 | 8  | 5492 | OWO | WAT | V | 39 | 31.355 | 60.893 | 19.838 | 1.00 | 12.31 | 8 |
| 5451 | CA  | WAT | A | 692 | 32.693 | 60.307 | 13.017 | 1.00 | 11.99 | 20 | 5493 | OWO | WAT | V | 40 | 16.930 | 64.546 | 40.981 | 1.00 | 12.36 | 8 |
| 5452 | CA  | WAT | A | 693 | 26.975 | 79.502 | 21.970 | 1.00 | 10.73 | 20 | 5494 | OWO | WAT | V | 41 | 10.918 | 81.011 | 32.425 | 1.00 | 12.42 | 8 |
| 5453 | CA  | WAT | A | 694 | 37.244 | 49.841 | 19.039 | 1.00 | 13.50 | 20 | 5495 | OWO | WAT | V | 42 | 8.358  | 78.559 | 35.685 | 1.00 | 12.49 | 8 |
| 5454 | OWO | WAT | V | 1   | 24.447 | 79.971 | 21.858 | 1.00 | 9.43  | 8  | 5496 | OWO | WAT | V | 43 | 22.052 | 71.621 | 41.190 | 1.00 | 12.24 | 8 |
| 5455 | OWO | WAT | V | 2   | 35.686 | 59.385 | 24.028 | 1.00 | 10.45 | 8  | 5497 | OWO | WAT | V | 44 | 8.226  | 66.640 | 35.276 | 1.00 | 12.62 | 8 |
| 5456 | OWO | WAT | V | 3   | 33.934 | 60.773 | 18.648 | 1.00 | 10.63 | 8  | 5498 | OWO | WAT | V | 45 | 6.031  | 77.562 | 36.868 | 1.00 | 12.35 | 8 |
| 5457 | OWO | WAT | V | 4   | 35.622 | 62.751 | 41.495 | 1.00 | 10.88 | 8  | 5499 | OWO | WAT | V | 46 | 43.919 | 60.734 | 40.175 | 1.00 | 12.51 | 8 |
| 5458 | OWO | WAT | V | 5   | 25.780 | 77.914 | 20.486 | 1.00 | 10.75 | 8  | 5500 | OWO | WAT | V | 48 | 11.578 | 73.478 | 41.191 | 1.00 | 12.62 | 8 |
| 5459 | OWO | WAT | V | 6   | 21.776 | 77.285 | 28.879 | 1.00 | 10.81 | 8  | 5501 | OWO | WAT | V | 49 | 35.256 | 52.308 | 26.203 | 1.00 | 12.50 | 8 |
| 5460 | OWO | WAT | V | 7   | 29.415 | 69.145 | 19.400 | 1.00 | 10.86 | 8  | 5502 | OWO | WAT | V | 50 | 22.628 | 81.739 | 22.782 | 1.00 | 12.52 | 8 |
| 5461 | OWO | WAT | V | 8   | 29.138 | 80.312 | 22.631 | 1.00 | 10.86 | 8  | 5503 | OWO | WAT | V | 51 | 41.171 | 68.357 | 22.292 | 1.00 | 12.78 | 8 |
| 5462 | OWO | WAT | V | 9   | 27.613 | 72.037 | 24.448 | 1.00 | 10.77 | 8  | 5504 | OWO | WAT | V | 52 | 34.554 | 71.110 | 10.783 | 1.00 | 12.58 | 8 |
| 5463 | OWO | WAT | V | 10  | 31.164 | 77.784 | 19.615 | 1.00 | 10.85 | 8  | 5505 | OWO | WAT | V | 53 | 39.554 | 70.543 | 28.407 | 1.00 | 12.73 | 8 |
| 5464 | OWO | WAT | V | 11  | 32.790 | 66.917 | 36.378 | 1.00 | 10.94 | 8  | 5506 | OWO | WAT | V | 54 | 14.970 | 66.671 | 43.779 | 1.00 | 12.94 | 8 |
| 5465 | OWO | WAT | V | 12  | 34.127 | 70.240 | 32.929 | 1.00 | 11.18 | 8  | 5507 | OWO | WAT | V | 55 | 14.792 | 81.581 | 20.763 | 1.00 | 12.92 | 8 |
| 5466 | OWO | WAT | V | 13  | 33.080 | 60.581 | 23.767 | 1.00 | 11.11 | 8  | 5508 | OWO | WAT | V | 56 | 30.205 | 75.643 | 31.109 | 1.00 | 12.90 | 8 |
| 5467 | OWO | WAT | V | 14  | 37.235 | 54.601 | 19.600 | 1.00 | 11.38 | 8  | 5509 | OWO | WAT | V | 57 | 16.697 | 82.536 | 30.534 | 1.00 | 13.09 | 8 |
| 5468 | OWO | WAT | V | 15  | 26.119 | 65.542 | 21.574 | 1.00 | 11.07 | 8  | 5510 | OWO | WAT | V | 58 | 38.776 | 53.289 | 57.732 | 1.00 | 13.10 | 8 |
| 5469 | OWO | WAT | V | 16  | 28.484 | 64.486 | 20.522 | 1.00 | 11.49 | 8  | 5511 | OWO | WAT | V | 59 | 31.555 | 49.273 | 20.064 | 1.00 | 13.22 | 8 |
| 5470 | OWO | WAT | V | 17  | 28.194 | 73.536 | 36.853 | 1.00 | 11.53 | 8  | 5512 | OWO | WAT | V | 60 | 20.200 | 85.147 | 36.037 | 1.00 | 13.29 | 8 |
| 5471 | OWO | WAT | V | 18  | 16.618 | 66.275 | 36.806 | 1.00 | 11.68 | 8  | 5513 | OWO | WAT | V | 61 | 25.657 | 54.513 | 45.949 | 1.00 | 13.32 | 8 |

|      |     |     |   |     |        |        |        |      |       |   |      |     |     |   |     |        |         |        |      |       |   |
|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| 5514 | OWO | WAT | V | 62  | 37.048 | 52.273 | 18.284 | 1.00 | 13.46 | 8 | 5556 | OWO | WAT | V | 104 | 14.144 | 58.009  | 41.510 | 1.00 | 15.84 | 8 |
| 5515 | OWO | WAT | V | 63  | 30.032 | 67.305 | 53.938 | 1.00 | 13.27 | 8 | 5557 | OWO | WAT | V | 105 | 44.010 | 71.623  | 35.990 | 1.00 | 15.89 | 8 |
| 5516 | OWO | WAT | V | 64  | 32.331 | 68.357 | 33.829 | 1.00 | 13.58 | 8 | 5558 | OWO | WAT | V | 106 | 21.168 | 82.474  | 32.738 | 1.00 | 16.12 | 8 |
| 5517 | OWO | WAT | V | 65  | 23.329 | 85.511 | 30.252 | 1.00 | 13.33 | 8 | 5559 | OWO | WAT | V | 107 | 28.667 | 48.688  | 46.155 | 1.00 | 16.35 | 8 |
| 5518 | OWO | WAT | V | 66  | 20.246 | 61.387 | 18.981 | 1.00 | 13.61 | 8 | 5560 | OWO | WAT | V | 108 | 25.610 | 86.818  | 38.209 | 1.00 | 16.18 | 8 |
| 5519 | OWO | WAT | V | 67  | 28.775 | 74.856 | 40.336 | 1.00 | 13.65 | 8 | 5561 | OWO | WAT | V | 109 | 29.070 | 89.992  | 31.492 | 1.00 | 16.47 | 8 |
| 5520 | OWO | WAT | V | 68  | 32.567 | 68.924 | 43.607 | 1.00 | 13.35 | 8 | 5562 | OWO | WAT | V | 110 | 1.291  | 75.000  | 41.091 | 1.00 | 16.32 | 8 |
| 5521 | OWO | WAT | V | 69  | 10.838 | 68.713 | 42.880 | 1.00 | 13.33 | 8 | 5563 | OWO | WAT | V | 111 | 34.624 | 56.600  | 71.328 | 1.00 | 16.34 | 8 |
| 5522 | OWO | WAT | V | 70  | 12.859 | 61.518 | 43.606 | 1.00 | 13.90 | 8 | 5564 | OWO | WAT | V | 112 | 28.281 | 69.481  | 68.152 | 1.00 | 16.52 | 8 |
| 5523 | OWO | WAT | V | 71  | 45.207 | 60.214 | 32.334 | 1.00 | 13.77 | 8 | 5565 | OWO | WAT | V | 113 | 26.135 | 87.038  | 35.304 | 1.00 | 16.58 | 8 |
| 5524 | OWO | WAT | V | 72  | 27.427 | 66.987 | 53.108 | 1.00 | 13.75 | 8 | 5566 | OWO | WAT | V | 114 | 35.168 | 78.123  | 51.153 | 1.00 | 16.64 | 8 |
| 5525 | OWO | WAT | V | 73  | 19.074 | 63.276 | 42.264 | 1.00 | 13.66 | 8 | 5567 | OWO | WAT | V | 115 | 19.827 | 81.281  | 46.203 | 1.00 | 16.48 | 8 |
| 5526 | OWO | WAT | V | 74  | 36.934 | 75.592 | 8.270  | 1.00 | 13.53 | 8 | 5568 | OWO | WAT | V | 116 | 30.082 | 84.087  | 8.323  | 1.00 | 16.75 | 8 |
| 5527 | OWO | WAT | V | 75  | 27.574 | 81.410 | 6.013  | 1.00 | 14.19 | 8 | 5569 | OWO | WAT | V | 117 | 45.164 | 71.238  | 15.992 | 1.00 | 16.58 | 8 |
| 5528 | OWO | WAT | V | 76  | 30.621 | 83.670 | 31.215 | 1.00 | 14.28 | 8 | 5570 | OWO | WAT | V | 118 | -2.555 | 86.829  | 29.585 | 1.00 | 16.73 | 8 |
| 5529 | OWO | WAT | V | 77  | 42.514 | 70.356 | 20.822 | 1.00 | 14.45 | 8 | 5571 | OWO | WAT | V | 119 | 1.879  | 75.860  | 26.297 | 1.00 | 16.96 | 8 |
| 5530 | OWO | WAT | V | 78  | 12.529 | 75.168 | 22.815 | 1.00 | 14.52 | 8 | 5572 | OWO | WAT | V | 120 | 20.960 | 94.415  | 22.713 | 1.00 | 16.87 | 8 |
| 5531 | OWO | WAT | V | 79  | 39.891 | 56.461 | 11.992 | 1.00 | 14.18 | 8 | 5573 | OWO | WAT | V | 121 | 12.300 | 72.626  | 21.951 | 1.00 | 16.94 | 8 |
| 5532 | OWO | WAT | V | 80  | 30.677 | 68.114 | 68.620 | 1.00 | 14.47 | 8 | 5574 | OWO | WAT | V | 122 | 21.720 | 86.954  | 37.648 | 1.00 | 17.08 | 8 |
| 5533 | OWO | WAT | V | 81  | 33.218 | 64.224 | 36.711 | 1.00 | 14.46 | 8 | 5575 | OWO | WAT | V | 123 | 17.342 | 46.052  | 29.967 | 1.00 | 16.89 | 8 |
| 5534 | OWO | WAT | V | 82  | 12.035 | 74.811 | 37.533 | 1.00 | 14.63 | 8 | 5576 | OWO | WAT | V | 124 | 15.847 | 84.337  | 34.562 | 1.00 | 16.74 | 8 |
| 5535 | OWO | WAT | V | 83  | 15.981 | 73.538 | 38.569 | 1.00 | 14.16 | 8 | 5577 | OWO | WAT | V | 125 | -3.241 | 60.294  | 45.682 | 1.00 | 16.67 | 8 |
| 5536 | OWO | WAT | V | 84  | 10.686 | 81.113 | 35.947 | 1.00 | 14.90 | 8 | 5578 | OWO | WAT | V | 126 | 11.587 | 104.148 | 24.323 | 1.00 | 17.24 | 8 |
| 5537 | OWO | WAT | V | 85  | 25.562 | 71.871 | 51.287 | 1.00 | 14.81 | 8 | 5579 | OWO | WAT | V | 127 | 28.501 | 56.852  | 51.441 | 1.00 | 17.40 | 8 |
| 5538 | OWO | WAT | V | 86  | 29.447 | 83.564 | 16.644 | 1.00 | 14.86 | 8 | 5580 | OWO | WAT | V | 128 | 14.206 | 82.937  | 18.392 | 1.00 | 17.22 | 8 |
| 5539 | OWO | WAT | V | 87  | 13.480 | 81.300 | 31.112 | 1.00 | 14.85 | 8 | 5581 | OWO | WAT | V | 129 | 41.516 | 56.407  | 63.525 | 1.00 | 17.65 | 8 |
| 5540 | OWO | WAT | V | 88  | 5.774  | 80.076 | 41.775 | 1.00 | 14.92 | 8 | 5582 | OWO | WAT | V | 130 | 36.936 | 73.986  | 40.016 | 1.00 | 17.53 | 8 |
| 5541 | OWO | WAT | V | 89  | 47.914 | 63.828 | 68.644 | 1.00 | 14.87 | 8 | 5583 | OWO | WAT | V | 131 | 20.790 | 40.115  | 27.752 | 1.00 | 17.55 | 8 |
| 5542 | OWO | WAT | V | 90  | 34.743 | 77.662 | 45.101 | 1.00 | 15.02 | 8 | 5584 | OWO | WAT | V | 132 | 45.240 | 52.146  | 20.212 | 1.00 | 17.29 | 8 |
| 5543 | OWO | WAT | V | 91  | 24.427 | 76.387 | 7.359  | 1.00 | 15.03 | 8 | 5585 | OWO | WAT | V | 133 | 41.799 | 49.726  | 28.892 | 1.00 | 17.29 | 8 |
| 5544 | OWO | WAT | V | 92  | -2.703 | 63.471 | 38.845 | 1.00 | 15.46 | 8 | 5586 | OWO | WAT | V | 134 | 23.108 | 66.755  | 60.083 | 1.00 | 17.41 | 8 |
| 5545 | OWO | WAT | V | 93  | 14.681 | 69.092 | 37.625 | 1.00 | 15.14 | 8 | 5587 | OWO | WAT | V | 135 | 26.863 | 48.805  | 41.435 | 1.00 | 17.67 | 8 |
| 5546 | OWO | WAT | V | 94  | 28.123 | 74.474 | 42.954 | 1.00 | 15.12 | 8 | 5588 | OWO | WAT | V | 136 | 27.488 | 90.699  | 28.339 | 1.00 | 17.76 | 8 |
| 5547 | OWO | WAT | V | 95  | 23.589 | 80.407 | 29.737 | 1.00 | 15.19 | 8 | 5589 | OWO | WAT | V | 137 | 0.191  | 69.111  | 49.096 | 1.00 | 17.78 | 8 |
| 5548 | OWO | WAT | V | 96  | 28.941 | 64.658 | 47.281 | 1.00 | 15.32 | 8 | 5590 | OWO | WAT | V | 138 | 34.447 | 43.232  | 33.946 | 1.00 | 17.85 | 8 |
| 5549 | OWO | WAT | V | 97  | 33.848 | 82.923 | 7.441  | 1.00 | 15.09 | 8 | 5591 | OWO | WAT | V | 139 | 22.589 | 64.044  | 49.415 | 1.00 | 18.18 | 8 |
| 5550 | OWO | WAT | V | 98  | 50.687 | 59.709 | 65.034 | 1.00 | 15.32 | 8 | 5592 | OWO | WAT | V | 140 | 17.697 | 81.339  | 35.462 | 1.00 | 17.98 | 8 |
| 5551 | OWO | WAT | V | 99  | 29.977 | 80.264 | 14.804 | 1.00 | 15.36 | 8 | 5593 | OWO | WAT | V | 141 | 2.444  | 96.838  | 37.934 | 1.00 | 18.09 | 8 |
| 5552 | OWO | WAT | V | 100 | 25.916 | 52.607 | 44.011 | 1.00 | 15.58 | 8 | 5594 | OWO | WAT | V | 142 | 35.347 | 81.251  | 39.545 | 1.00 | 17.94 | 8 |
| 5553 | OWO | WAT | V | 101 | 6.765  | 62.176 | 32.083 | 1.00 | 15.56 | 8 | 5595 | OWO | WAT | V | 143 | 14.511 | 56.297  | 49.652 | 1.00 | 18.35 | 8 |
| 5554 | OWO | WAT | V | 102 | 13.107 | 89.810 | 20.076 | 1.00 | 15.94 | 8 | 5596 | OWO | WAT | V | 144 | 10.014 | 71.654  | 20.618 | 1.00 | 18.11 | 8 |
| 5555 | OWO | WAT | V | 103 | 11.601 | 78.292 | 36.745 | 1.00 | 15.75 | 8 | 5597 | OWO | WAT | V | 145 | 47.629 | 63.815  | 18.991 | 1.00 | 18.25 | 8 |

|      |               |        |         |        |            |   |      |               |        |        |        |            |   |
|------|---------------|--------|---------|--------|------------|---|------|---------------|--------|--------|--------|------------|---|
| 5598 | OWO WAT V 146 | 15.832 | 79.962  | 31.635 | 1.00 18.52 | 8 | 5640 | OWO WAT V 195 | 43.898 | 69.204 | 9.296  | 1.00 20.35 | 8 |
| 5599 | OWO WAT V 147 | 35.482 | 76.428  | 39.594 | 1.00 18.64 | 8 | 5641 | OWO WAT V 196 | 17.503 | 91.553 | 19.944 | 1.00 20.36 | 8 |
| 5600 | OWO WAT V 149 | 16.532 | 67.334  | 48.159 | 1.00 18.61 | 8 | 5642 | OWO WAT V 197 | 22.079 | 71.014 | 56.203 | 1.00 20.50 | 8 |
| 5601 | OWO WAT V 150 | 32.280 | 83.173  | 33.550 | 1.00 18.44 | 8 | 5643 | OWO WAT V 198 | 24.611 | 90.278 | 32.659 | 1.00 20.71 | 8 |
| 5602 | OWO WAT V 151 | 35.037 | 62.885  | 71.628 | 1.00 18.62 | 8 | 5644 | OWO WAT V 199 | 15.822 | 79.667 | 34.285 | 1.00 20.71 | 8 |
| 5603 | OWO WAT V 152 | 14.756 | 56.448  | 28.743 | 1.00 18.87 | 8 | 5645 | OWO WAT V 200 | 41.507 | 64.519 | 35.769 | 1.00 20.47 | 8 |
| 5604 | OWO WAT V 153 | 51.007 | 64.138  | 32.515 | 1.00 18.45 | 8 | 5646 | OWO WAT V 201 | 50.582 | 63.510 | 21.444 | 1.00 20.44 | 8 |
| 5605 | OWO WAT V 154 | 44.683 | 55.406  | 52.749 | 1.00 18.86 | 8 | 5647 | OWO WAT V 202 | -4.254 | 88.781 | 28.481 | 1.00 20.69 | 8 |
| 5606 | OWO WAT V 155 | 30.803 | 47.286  | 18.413 | 1.00 19.00 | 8 | 5648 | OWO WAT V 203 | 41.289 | 48.120 | 25.349 | 1.00 20.50 | 8 |
| 5607 | OWO WAT V 156 | 21.419 | 87.008  | 31.586 | 1.00 18.86 | 8 | 5649 | OWO WAT V 204 | 33.838 | 47.522 | 55.491 | 1.00 20.42 | 8 |
| 5608 | OWO WAT V 157 | 27.471 | 54.562  | 13.822 | 1.00 18.86 | 8 | 5650 | OWO WAT V 205 | 28.696 | 42.611 | 30.481 | 1.00 21.10 | 8 |
| 5609 | OWO WAT V 158 | 19.938 | 85.031  | 32.888 | 1.00 18.77 | 8 | 5651 | OWO WAT V 206 | 29.680 | 89.479 | 34.207 | 1.00 20.71 | 8 |
| 5610 | OWO WAT V 160 | 23.159 | 58.927  | 72.012 | 1.00 19.01 | 8 | 5652 | OWO WAT V 207 | 13.375 | 82.989 | 38.528 | 1.00 20.79 | 8 |
| 5611 | OWO WAT V 161 | 20.470 | 84.773  | 18.243 | 1.00 19.09 | 8 | 5653 | OWO WAT V 208 | -0.381 | 94.652 | 35.925 | 1.00 20.71 | 8 |
| 5612 | OWO WAT V 162 | 15.077 | 66.831  | 13.792 | 1.00 18.88 | 8 | 5654 | OWO WAT V 209 | 32.894 | 53.249 | 7.401  | 1.00 20.79 | 8 |
| 5613 | OWO WAT V 164 | 34.016 | 76.548  | 58.886 | 1.00 19.18 | 8 | 5655 | OWO WAT V 210 | 47.202 | 71.009 | 63.961 | 1.00 20.83 | 8 |
| 5614 | OWO WAT V 165 | 1.791  | 96.077  | 35.490 | 1.00 19.39 | 8 | 5656 | OWO WAT V 211 | 16.432 | 73.589 | 49.935 | 1.00 20.64 | 8 |
| 5615 | OWO WAT V 168 | 16.921 | 65.681  | 50.173 | 1.00 19.74 | 8 | 5657 | OWO WAT V 212 | 36.761 | 42.123 | 23.718 | 1.00 20.49 | 8 |
| 5616 | OWO WAT V 169 | 36.015 | 49.508  | 63.823 | 1.00 19.75 | 8 | 5658 | OWO WAT V 213 | 1.326  | 98.176 | 25.977 | 1.00 21.14 | 8 |
| 5617 | OWO WAT V 170 | 19.146 | 93.639  | 20.716 | 1.00 19.72 | 8 | 5659 | OWO WAT V 215 | 32.369 | 84.143 | 13.694 | 1.00 21.27 | 8 |
| 5618 | OWO WAT V 171 | 41.081 | 74.262  | 43.114 | 1.00 19.99 | 8 | 5660 | OWO WAT V 216 | 1.000  | 72.006 | 27.168 | 1.00 21.23 | 8 |
| 5619 | OWO WAT V 172 | 27.356 | 86.834  | 41.150 | 1.00 19.86 | 8 | 5661 | OWO WAT V 217 | 21.907 | 50.669 | 62.000 | 1.00 21.19 | 8 |
| 5620 | OWO WAT V 173 | 32.541 | 61.241  | 6.239  | 1.00 19.49 | 8 | 5662 | OWO WAT V 218 | 30.956 | 41.738 | 21.314 | 1.00 21.03 | 8 |
| 5621 | OWO WAT V 174 | 51.971 | 65.011  | 17.317 | 1.00 20.07 | 8 | 5663 | OWO WAT V 219 | 36.121 | 71.463 | 4.684  | 1.00 21.46 | 8 |
| 5622 | OWO WAT V 175 | 36.754 | 79.161  | 49.332 | 1.00 19.96 | 8 | 5664 | OWO WAT V 220 | 13.404 | 81.016 | 34.970 | 1.00 21.65 | 8 |
| 5623 | OWO WAT V 176 | 21.529 | 68.516  | 52.600 | 1.00 19.88 | 8 | 5665 | OWO WAT V 221 | 22.957 | 65.844 | 62.604 | 1.00 21.35 | 8 |
| 5624 | OWO WAT V 177 | 52.175 | 64.476  | 48.627 | 1.00 19.48 | 8 | 5666 | OWO WAT V 222 | 4.260  | 99.337 | 39.649 | 1.00 21.63 | 8 |
| 5625 | OWO WAT V 178 | 47.687 | 55.894  | 28.556 | 1.00 19.85 | 8 | 5667 | OWO WAT V 223 | 17.535 | 84.263 | 32.555 | 1.00 20.98 | 8 |
| 5626 | OWO WAT V 180 | 28.309 | 57.733  | 12.302 | 1.00 19.86 | 8 | 5668 | OWO WAT V 224 | 16.496 | 59.065 | 45.746 | 1.00 21.66 | 8 |
| 5627 | OWO WAT V 181 | 19.852 | 88.585  | 39.017 | 1.00 20.03 | 8 | 5669 | OWO WAT V 225 | 16.576 | 52.574 | 34.164 | 1.00 21.65 | 8 |
| 5628 | OWO WAT V 182 | 48.116 | 65.053  | 11.253 | 1.00 19.75 | 8 | 5670 | OWO WAT V 226 | 30.825 | 51.406 | 13.432 | 1.00 21.28 | 8 |
| 5629 | OWO WAT V 183 | 45.728 | 49.401  | 46.755 | 1.00 20.07 | 8 | 5671 | OWO WAT V 227 | 39.177 | 82.848 | 23.121 | 1.00 21.63 | 8 |
| 5630 | OWO WAT V 184 | 23.090 | 51.403  | 56.173 | 1.00 19.76 | 8 | 5672 | OWO WAT V 229 | 19.108 | 58.790 | 36.143 | 1.00 21.40 | 8 |
| 5631 | OWO WAT V 185 | 23.972 | 69.604  | 53.226 | 1.00 20.10 | 8 | 5673 | OWO WAT V 230 | 19.087 | 75.378 | 50.063 | 1.00 21.22 | 8 |
| 5632 | OWO WAT V 186 | 49.679 | 65.500  | 55.245 | 1.00 19.98 | 8 | 5674 | OWO WAT V 231 | 47.413 | 69.881 | 16.583 | 1.00 21.29 | 8 |
| 5633 | OWO WAT V 187 | 50.720 | 57.388  | 48.688 | 1.00 20.39 | 8 | 5675 | OWO WAT V 232 | 26.686 | 91.040 | 31.058 | 1.00 21.61 | 8 |
| 5634 | OWO WAT V 188 | 34.857 | 63.152  | 38.228 | 1.00 20.23 | 8 | 5676 | OWO WAT V 233 | 29.036 | 52.089 | 61.852 | 1.00 21.25 | 8 |
| 5635 | OWO WAT V 189 | 37.511 | 43.029  | 19.233 | 1.00 20.32 | 8 | 5677 | OWO WAT V 234 | 36.187 | 79.293 | 46.671 | 1.00 21.45 | 8 |
| 5636 | OWO WAT V 190 | 50.567 | 67.974  | 10.449 | 1.00 20.64 | 8 | 5678 | OWO WAT V 235 | 37.289 | 74.835 | 65.582 | 1.00 21.65 | 8 |
| 5637 | OWO WAT V 191 | 29.875 | 92.014  | 24.922 | 1.00 20.34 | 8 | 5679 | OWO WAT V 236 | -0.428 | 68.770 | 30.109 | 1.00 21.94 | 8 |
| 5638 | OWO WAT V 192 | 4.055  | 100.811 | 36.567 | 1.00 20.35 | 8 | 5680 | OWO WAT V 237 | 50.762 | 57.829 | 44.061 | 1.00 22.15 | 8 |
| 5639 | OWO WAT V 194 | 23.592 | 87.859  | 32.780 | 1.00 20.02 | 8 | 5681 | OWO WAT V 238 | 45.167 | 70.565 | 24.893 | 1.00 22.00 | 8 |

Table 1. Summary of the results of the analysis of variance for the effect of the treatment on the response of the subjects to the test. The results are presented in the form of a table with the following columns: Treatment, Response, and F-value. The F-value is the ratio of the mean square for the treatment to the mean square for the error. The results are presented in the form of a table with the following columns: Treatment, Response, and F-value.

|      |               |        |         |        |            |   |      |               |        |         |        |            |   |
|------|---------------|--------|---------|--------|------------|---|------|---------------|--------|---------|--------|------------|---|
| 5682 | OWO WAT V 239 | 28.609 | 48.609  | 51.930 | 1.00 22.03 | 8 | 5724 | OWO WAT V 282 | 13.480 | 62.142  | 18.325 | 1.00 23.48 | 8 |
| 5683 | OWO WAT V 241 | 2.366  | 94.552  | 38.603 | 1.00 21.97 | 8 | 5725 | OWO WAT V 283 | 19.332 | 56.925  | 43.429 | 1.00 23.84 | 8 |
| 5684 | OWO WAT V 242 | 9.365  | 68.970  | 20.742 | 1.00 22.04 | 8 | 5726 | OWO WAT V 284 | 7.117  | 53.127  | 42.902 | 1.00 23.57 | 8 |
| 5685 | OWO WAT V 243 | 38.583 | 85.642  | 29.447 | 1.00 21.90 | 8 | 5727 | OWO WAT V 285 | 27.829 | 78.220  | 46.852 | 1.00 24.20 | 8 |
| 5686 | OWO WAT V 244 | 24.639 | 49.542  | 55.081 | 1.00 22.42 | 8 | 5728 | OWO WAT V 286 | 49.295 | 57.105  | 51.124 | 1.00 23.77 | 8 |
| 5687 | OWO WAT V 245 | 18.177 | 95.474  | 18.838 | 1.00 22.69 | 8 | 5729 | OWO WAT V 287 | 13.680 | 105.356 | 27.022 | 1.00 24.03 | 8 |
| 5688 | OWO WAT V 246 | 37.307 | 43.276  | 33.862 | 1.00 22.90 | 8 | 5730 | OWO WAT V 288 | 17.824 | 106.639 | 32.939 | 1.00 24.44 | 8 |
| 5689 | OWO WAT V 247 | 23.478 | 86.290  | 16.425 | 1.00 21.85 | 8 | 5731 | OWO WAT V 289 | 15.542 | 66.715  | 53.507 | 1.00 24.42 | 8 |
| 5690 | OWO WAT V 248 | 43.569 | 60.466  | 72.156 | 1.00 23.10 | 8 | 5732 | OWO WAT V 290 | 27.050 | 47.324  | 23.573 | 1.00 24.19 | 8 |
| 5691 | OWO WAT V 249 | 23.281 | 40.658  | 26.691 | 1.00 22.77 | 8 | 5733 | OWO WAT V 291 | 39.482 | 73.577  | 31.816 | 1.00 24.19 | 8 |
| 5692 | OWO WAT V 250 | 8.761  | 65.837  | 24.376 | 1.00 23.00 | 8 | 5734 | OWO WAT V 292 | 10.356 | 77.638  | 16.052 | 1.00 23.96 | 8 |
| 5693 | OWO WAT V 251 | 27.215 | 72.803  | 60.509 | 1.00 22.60 | 8 | 5735 | OWO WAT V 293 | 24.405 | 50.730  | 63.252 | 1.00 24.31 | 8 |
| 5694 | OWO WAT V 252 | 16.174 | 91.014  | 44.772 | 1.00 22.53 | 8 | 5736 | OWO WAT V 294 | 15.639 | 54.776  | 31.091 | 1.00 24.31 | 8 |
| 5695 | OWO WAT V 253 | 3.297  | 98.395  | 35.969 | 1.00 23.15 | 8 | 5737 | OWO WAT V 295 | -5.196 | 74.449  | 41.013 | 1.00 24.22 | 8 |
| 5696 | OWO WAT V 254 | 10.918 | 68.974  | 53.447 | 1.00 23.22 | 8 | 5738 | OWO WAT V 296 | 40.985 | 72.335  | 29.872 | 1.00 24.55 | 8 |
| 5697 | OWO WAT V 255 | -5.802 | 66.167  | 37.375 | 1.00 23.15 | 8 | 5739 | OWO WAT V 297 | 48.449 | 77.051  | 18.858 | 1.00 24.18 | 8 |
| 5698 | OWO WAT V 256 | 8.490  | 91.603  | 44.099 | 1.00 22.65 | 8 | 5740 | OWO WAT V 298 | 25.992 | 92.521  | 26.784 | 1.00 24.84 | 8 |
| 5699 | OWO WAT V 257 | 9.234  | 73.507  | 16.552 | 1.00 22.92 | 8 | 5741 | OWO WAT V 299 | 45.814 | 49.306  | 39.112 | 1.00 24.65 | 8 |
| 5700 | OWO WAT V 258 | 15.730 | 56.257  | 16.556 | 1.00 23.08 | 8 | 5742 | OWO WAT V 300 | 44.725 | 55.968  | 11.440 | 1.00 24.94 | 8 |
| 5701 | OWO WAT V 259 | 19.989 | 82.268  | 13.713 | 1.00 22.90 | 8 | 5743 | OWO WAT V 301 | 20.058 | 84.809  | 46.357 | 1.00 24.73 | 8 |
| 5702 | OWO WAT V 260 | 27.613 | 49.792  | 60.562 | 1.00 23.09 | 8 | 5744 | OWO WAT V 302 | 18.079 | 50.984  | 17.334 | 1.00 24.58 | 8 |
| 5703 | OWO WAT V 261 | 26.408 | 61.061  | 10.006 | 1.00 23.11 | 8 | 5745 | OWO WAT V 303 | 17.020 | 65.666  | 56.879 | 1.00 24.81 | 8 |
| 5704 | OWO WAT V 262 | 14.277 | 70.834  | 12.781 | 1.00 23.32 | 8 | 5746 | OWO WAT V 304 | 44.682 | 72.661  | 22.319 | 1.00 24.66 | 8 |
| 5705 | OWO WAT V 263 | -3.969 | 72.948  | 34.601 | 1.00 22.98 | 8 | 5747 | OWO WAT V 305 | 0.091  | 75.457  | 45.401 | 1.00 24.37 | 8 |
| 5706 | OWO WAT V 264 | -1.028 | 93.829  | 38.475 | 1.00 23.17 | 8 | 5748 | OWO WAT V 306 | 50.222 | 58.393  | 53.380 | 1.00 24.90 | 8 |
| 5707 | OWO WAT V 265 | 19.230 | 101.476 | 27.805 | 1.00 22.95 | 8 | 5749 | OWO WAT V 307 | 44.639 | 52.674  | 53.486 | 1.00 25.29 | 8 |
| 5708 | OWO WAT V 266 | 17.914 | 54.281  | 55.523 | 1.00 23.31 | 8 | 5750 | OWO WAT V 308 | 49.725 | 64.827  | 52.493 | 1.00 24.60 | 8 |
| 5709 | OWO WAT V 267 | -1.163 | 64.024  | 50.895 | 1.00 23.41 | 8 | 5751 | OWO WAT V 309 | 39.542 | 61.118  | 7.698  | 1.00 24.82 | 8 |
| 5710 | OWO WAT V 268 | 16.209 | 48.607  | 29.481 | 1.00 23.45 | 8 | 5752 | OWO WAT V 310 | 41.190 | 79.148  | 23.073 | 1.00 25.15 | 8 |
| 5711 | OWO WAT V 269 | 35.070 | 63.595  | 75.008 | 1.00 23.90 | 8 | 5753 | OWO WAT V 311 | 1.598  | 80.899  | 39.623 | 1.00 24.95 | 8 |
| 5712 | OWO WAT V 270 | 38.343 | 43.626  | 21.918 | 1.00 23.33 | 8 | 5754 | OWO WAT V 312 | 25.053 | 45.139  | 19.817 | 1.00 24.92 | 8 |
| 5713 | OWO WAT V 271 | 32.197 | 85.153  | 37.181 | 1.00 23.49 | 8 | 5755 | OWO WAT V 313 | 16.135 | 84.191  | 47.663 | 1.00 25.20 | 8 |
| 5714 | OWO WAT V 272 | 28.789 | 71.419  | 66.331 | 1.00 22.79 | 8 | 5756 | OWO WAT V 314 | 11.381 | 71.857  | 49.110 | 1.00 25.29 | 8 |
| 5715 | OWO WAT V 273 | 41.806 | 79.697  | 18.591 | 1.00 23.39 | 8 | 5757 | OWO WAT V 315 | -4.512 | 57.278  | 42.326 | 1.00 25.43 | 8 |
| 5716 | OWO WAT V 274 | 38.127 | 43.105  | 36.443 | 1.00 23.39 | 8 | 5758 | OWO WAT V 316 | 3.805  | 93.061  | 22.790 | 1.00 25.09 | 8 |
| 5717 | OWO WAT V 275 | 16.104 | 65.021  | 59.364 | 1.00 23.44 | 8 | 5759 | OWO WAT V 317 | 34.832 | 82.782  | 37.221 | 1.00 25.16 | 8 |
| 5718 | OWO WAT V 276 | -6.314 | 69.710  | 39.367 | 1.00 24.17 | 8 | 5760 | OWO WAT V 318 | 3.711  | 95.706  | 23.179 | 1.00 25.31 | 8 |
| 5719 | OWO WAT V 277 | 25.476 | 86.458  | 13.742 | 1.00 23.04 | 8 | 5761 | OWO WAT V 319 | 20.209 | 70.499  | 54.469 | 1.00 25.69 | 8 |
| 5720 | OWO WAT V 278 | 0.680  | 86.883  | 37.755 | 1.00 23.27 | 8 | 5762 | OWO WAT V 320 | 11.697 | 68.339  | 56.789 | 1.00 25.01 | 8 |
| 5721 | OWO WAT V 279 | 33.015 | 81.157  | 29.976 | 1.00 23.30 | 8 | 5763 | OWO WAT V 321 | 7.254  | 91.019  | 18.448 | 1.00 25.40 | 8 |
| 5722 | OWO WAT V 280 | 1.763  | 88.744  | 19.524 | 1.00 23.68 | 8 | 5764 | OWO WAT V 322 | 42.661 | 49.979  | 21.111 | 1.00 25.81 | 8 |
| 5723 | OWO WAT V 281 | 13.574 | 55.293  | 46.773 | 1.00 23.63 | 8 | 5765 | OWO WAT V 323 | 17.078 | 70.892  | 50.293 | 1.00 25.51 | 8 |

|      |     |     |   |     |        |         |        |      |       |   |      |     |     |   |     |        |         |        |      |       |   |
|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| 5766 | OWO | WAT | V | 324 | 49.200 | 60.915  | 31.600 | 1.00 | 25.53 | 8 | 5808 | OWO | WAT | V | 366 | 30.943 | 49.068  | 15.778 | 1.00 | 26.98 | 8 |
| 5767 | OWO | WAT | V | 325 | 31.661 | 71.214  | 4.552  | 1.00 | 25.64 | 8 | 5809 | OWO | WAT | V | 367 | 43.193 | 44.166  | 34.878 | 1.00 | 26.97 | 8 |
| 5768 | OWO | WAT | V | 326 | -2.062 | 96.310  | 27.990 | 1.00 | 25.87 | 8 | 5810 | OWO | WAT | V | 368 | 6.994  | 74.430  | 21.876 | 1.00 | 27.26 | 8 |
| 5769 | OWO | WAT | V | 327 | 39.125 | 80.230  | 56.164 | 1.00 | 26.25 | 8 | 5811 | OWO | WAT | V | 369 | 34.427 | 88.111  | 38.939 | 1.00 | 27.30 | 8 |
| 5770 | OWO | WAT | V | 328 | 48.433 | 70.294  | 57.525 | 1.00 | 25.87 | 8 | 5812 | OWO | WAT | V | 370 | 1.636  | 93.582  | 40.791 | 1.00 | 27.54 | 8 |
| 5771 | OWO | WAT | V | 329 | -2.772 | 64.990  | 34.941 | 1.00 | 25.71 | 8 | 5813 | OWO | WAT | V | 371 | 5.971  | 98.241  | 21.504 | 1.00 | 27.42 | 8 |
| 5772 | OWO | WAT | V | 330 | 35.352 | 40.001  | 22.353 | 1.00 | 25.96 | 8 | 5814 | OWO | WAT | V | 372 | 29.223 | 75.038  | 60.445 | 1.00 | 26.93 | 8 |
| 5773 | OWO | WAT | V | 331 | 34.557 | 81.627  | 46.792 | 1.00 | 26.23 | 8 | 5815 | OWO | WAT | V | 373 | 31.316 | 53.650  | 9.481  | 1.00 | 27.85 | 8 |
| 5774 | OWO | WAT | V | 332 | 23.250 | 92.581  | 31.676 | 1.00 | 26.20 | 8 | 5816 | OWO | WAT | V | 374 | 43.939 | 56.548  | 55.050 | 1.00 | 27.63 | 8 |
| 5775 | OWO | WAT | V | 333 | 23.167 | 53.251  | 13.715 | 1.00 | 25.74 | 8 | 5817 | OWO | WAT | V | 375 | 46.559 | 74.427  | 54.610 | 1.00 | 27.46 | 8 |
| 5776 | OWO | WAT | V | 334 | 20.707 | 52.356  | 39.202 | 1.00 | 25.65 | 8 | 5818 | OWO | WAT | V | 376 | 26.961 | 70.400  | 70.205 | 1.00 | 28.10 | 8 |
| 5777 | OWO | WAT | V | 335 | 4.870  | 93.727  | 41.264 | 1.00 | 26.54 | 8 | 5819 | OWO | WAT | V | 377 | 48.989 | 57.080  | 35.445 | 1.00 | 28.37 | 8 |
| 5778 | OWO | WAT | V | 336 | 0.053  | 71.401  | 29.885 | 1.00 | 25.67 | 8 | 5820 | OWO | WAT | V | 378 | 14.950 | 47.050  | 27.899 | 1.00 | 27.90 | 8 |
| 5779 | OWO | WAT | V | 337 | 20.015 | 56.517  | 72.324 | 1.00 | 25.86 | 8 | 5821 | OWO | WAT | V | 379 | 46.760 | 46.713  | 39.616 | 1.00 | 27.67 | 8 |
| 5780 | OWO | WAT | V | 338 | 13.826 | 74.132  | 49.507 | 1.00 | 26.36 | 8 | 5822 | OWO | WAT | V | 380 | -1.380 | 79.896  | 38.771 | 1.00 | 28.02 | 8 |
| 5781 | OWO | WAT | V | 339 | 44.958 | 71.632  | 28.685 | 1.00 | 26.80 | 8 | 5823 | OWO | WAT | V | 381 | 12.690 | 81.625  | 15.826 | 1.00 | 28.03 | 8 |
| 5782 | OWO | WAT | V | 340 | -0.093 | 73.784  | 33.119 | 1.00 | 26.07 | 8 | 5824 | OWO | WAT | V | 382 | 10.617 | 104.039 | 32.646 | 1.00 | 28.19 | 8 |
| 5783 | OWO | WAT | V | 341 | 49.630 | 56.579  | 40.106 | 1.00 | 26.64 | 8 | 5825 | OWO | WAT | V | 383 | 13.859 | 80.594  | 13.625 | 1.00 | 27.99 | 8 |
| 5784 | OWO | WAT | V | 342 | 15.628 | 79.186  | 45.524 | 1.00 | 26.42 | 8 | 5826 | OWO | WAT | V | 384 | 7.322  | 72.231  | 20.822 | 1.00 | 28.35 | 8 |
| 5785 | OWO | WAT | V | 343 | 31.176 | 91.867  | 30.769 | 1.00 | 26.10 | 8 | 5827 | OWO | WAT | V | 385 | 29.284 | 46.632  | 44.658 | 1.00 | 28.26 | 8 |
| 5786 | OWO | WAT | V | 344 | 15.626 | 67.643  | 55.543 | 1.00 | 26.46 | 8 | 5828 | OWO | WAT | V | 386 | 18.064 | 50.559  | 24.862 | 1.00 | 28.35 | 8 |
| 5787 | OWO | WAT | V | 345 | 21.398 | 95.678  | 38.839 | 1.00 | 26.79 | 8 | 5829 | OWO | WAT | V | 387 | 35.054 | 45.412  | 46.835 | 1.00 | 28.58 | 8 |
| 5788 | OWO | WAT | V | 346 | 41.099 | 41.982  | 39.915 | 1.00 | 26.66 | 8 | 5830 | OWO | WAT | V | 388 | 22.478 | 83.558  | 13.277 | 1.00 | 28.32 | 8 |
| 5789 | OWO | WAT | V | 347 | 22.442 | 79.888  | 2.661  | 1.00 | 26.18 | 8 | 5831 | OWO | WAT | V | 389 | 10.928 | 67.510  | 14.236 | 1.00 | 28.65 | 8 |
| 5790 | OWO | WAT | V | 348 | 44.448 | 72.532  | 39.099 | 1.00 | 27.08 | 8 | 5832 | OWO | WAT | V | 390 | 33.397 | 82.246  | 49.220 | 1.00 | 27.37 | 8 |
| 5791 | OWO | WAT | V | 349 | 40.265 | 82.719  | 10.175 | 1.00 | 26.27 | 8 | 5833 | OWO | WAT | V | 391 | 23.434 | 88.556  | 18.508 | 1.00 | 28.95 | 8 |
| 5792 | OWO | WAT | V | 350 | 40.934 | 43.657  | 30.662 | 1.00 | 27.04 | 8 | 5834 | OWO | WAT | V | 392 | 29.832 | 42.212  | 39.251 | 1.00 | 28.21 | 8 |
| 5793 | OWO | WAT | V | 351 | -1.666 | 97.213  | 32.163 | 1.00 | 27.31 | 8 | 5835 | OWO | WAT | V | 393 | 15.076 | 70.102  | 51.758 | 1.00 | 27.91 | 8 |
| 5794 | OWO | WAT | V | 352 | -8.111 | 67.221  | 45.293 | 1.00 | 27.12 | 8 | 5836 | OWO | WAT | V | 394 | 35.566 | 48.453  | 66.263 | 1.00 | 28.16 | 8 |
| 5795 | OWO | WAT | V | 353 | 16.355 | 56.614  | 42.471 | 1.00 | 27.10 | 8 | 5837 | OWO | WAT | V | 395 | 34.691 | 46.594  | 49.301 | 1.00 | 28.85 | 8 |
| 5796 | OWO | WAT | V | 354 | 11.346 | 65.531  | 19.934 | 1.00 | 27.40 | 8 | 5838 | OWO | WAT | V | 396 | 39.702 | 74.440  | 36.238 | 1.00 | 28.77 | 8 |
| 5797 | OWO | WAT | V | 355 | 11.189 | 105.275 | 21.949 | 1.00 | 27.29 | 8 | 5839 | OWO | WAT | V | 397 | 50.176 | 56.086  | 14.851 | 1.00 | 28.75 | 8 |
| 5798 | OWO | WAT | V | 356 | 23.545 | 83.502  | 8.615  | 1.00 | 27.06 | 8 | 5840 | OWO | WAT | V | 398 | 14.115 | 57.834  | 59.211 | 1.00 | 27.83 | 8 |
| 5799 | OWO | WAT | V | 357 | 22.122 | 49.913  | 14.384 | 1.00 | 27.06 | 8 | 5841 | OWO | WAT | V | 399 | 38.189 | 49.702  | 11.383 | 1.00 | 29.29 | 8 |
| 5800 | OWO | WAT | V | 358 | 6.833  | 52.668  | 34.000 | 1.00 | 27.79 | 8 | 5842 | OWO | WAT | V | 400 | 3.241  | 100.941 | 39.033 | 1.00 | 28.47 | 8 |
| 5801 | OWO | WAT | V | 359 | 30.479 | 47.598  | 56.666 | 1.00 | 27.66 | 8 | 5843 | OWO | WAT | V | 401 | 44.298 | 73.510  | 63.099 | 1.00 | 28.91 | 8 |
| 5802 | OWO | WAT | V | 360 | 33.166 | 42.826  | 19.802 | 1.00 | 27.33 | 8 | 5844 | OWO | WAT | V | 402 | 7.061  | 75.135  | 47.544 | 1.00 | 28.59 | 8 |
| 5803 | OWO | WAT | V | 361 | 24.029 | 55.851  | 13.947 | 1.00 | 28.08 | 8 | 5845 | OWO | WAT | V | 403 | 5.477  | 86.910  | 42.452 | 1.00 | 29.56 | 8 |
| 5804 | OWO | WAT | V | 362 | 39.488 | 85.709  | 20.632 | 1.00 | 27.01 | 8 | 5846 | OWO | WAT | V | 404 | 25.564 | 72.515  | 56.246 | 1.00 | 29.09 | 8 |
| 5805 | OWO | WAT | V | 363 | 2.130  | 49.916  | 43.049 | 1.00 | 27.26 | 8 | 5847 | OWO | WAT | V | 405 | 25.075 | 41.160  | 32.189 | 1.00 | 29.20 | 8 |
| 5806 | OWO | WAT | V | 364 | 35.616 | 41.373  | 27.626 | 1.00 | 27.13 | 8 | 5848 | OWO | WAT | V | 406 | 2.074  | 56.387  | 58.854 | 1.00 | 28.86 | 8 |
| 5807 | OWO | WAT | V | 365 | 50.664 | 58.560  | 41.450 | 1.00 | 26.59 | 8 | 5849 | OWO | WAT | V | 407 | 47.163 | 58.038  | 33.355 | 1.00 | 28.76 | 8 |

|      |               |        |         |        |            |   |      |               |        |         |        |            |   |
|------|---------------|--------|---------|--------|------------|---|------|---------------|--------|---------|--------|------------|---|
| 5850 | OWO WAT V 408 | 27.438 | 44.407  | 21.116 | 1.00 28.21 | 8 | 5892 | OWO WAT V 450 | 8.486  | 84.645  | 16.251 | 1.00 30.46 | 8 |
| 5851 | OWO WAT V 409 | 32.690 | 89.765  | 34.445 | 1.00 29.13 | 8 | 5893 | OWO WAT V 451 | 17.712 | 70.200  | 52.856 | 1.00 31.30 | 8 |
| 5852 | OWO WAT V 410 | 8.726  | 56.984  | 33.875 | 1.00 28.81 | 8 | 5894 | OWO WAT V 452 | 45.187 | 54.640  | 9.218  | 1.00 30.47 | 8 |
| 5853 | OWO WAT V 411 | -2.765 | 74.847  | 45.763 | 1.00 28.58 | 8 | 5895 | OWO WAT V 453 | 23.220 | 65.098  | 2.001  | 1.00 30.15 | 8 |
| 5854 | OWO WAT V 412 | 9.880  | 76.028  | 48.593 | 1.00 29.43 | 8 | 5896 | OWO WAT V 454 | 43.353 | 48.993  | 23.792 | 1.00 30.21 | 8 |
| 5855 | OWO WAT V 413 | 18.587 | 55.405  | 41.191 | 1.00 28.66 | 8 | 5897 | OWO WAT V 455 | 0.241  | 76.716  | 42.809 | 1.00 30.43 | 8 |
| 5856 | OWO WAT V 414 | 0.831  | 95.595  | 23.928 | 1.00 28.90 | 8 | 5898 | OWO WAT V 456 | 38.954 | 90.362  | 25.885 | 1.00 31.19 | 8 |
| 5857 | OWO WAT V 415 | 18.167 | 58.042  | 65.360 | 1.00 28.57 | 8 | 5899 | OWO WAT V 457 | 8.998  | 51.618  | 42.193 | 1.00 30.65 | 8 |
| 5858 | OWO WAT V 416 | 42.814 | 47.661  | 27.620 | 1.00 29.34 | 8 | 5900 | OWO WAT V 458 | 47.484 | 70.509  | 20.484 | 1.00 30.75 | 8 |
| 5859 | OWO WAT V 417 | 19.226 | 89.316  | 19.020 | 1.00 29.13 | 8 | 5901 | OWO WAT V 459 | 26.632 | 83.732  | 7.006  | 1.00 30.86 | 8 |
| 5860 | OWO WAT V 418 | 17.933 | 82.283  | 11.952 | 1.00 28.48 | 8 | 5902 | OWO WAT V 460 | 27.887 | 84.031  | 46.702 | 1.00 31.16 | 8 |
| 5861 | OWO WAT V 419 | 44.723 | 79.313  | 13.493 | 1.00 30.12 | 8 | 5903 | OWO WAT V 461 | 10.456 | 52.659  | 39.931 | 1.00 31.37 | 8 |
| 5862 | OWO WAT V 420 | 34.399 | 78.316  | 0.819  | 1.00 29.81 | 8 | 5904 | OWO WAT V 462 | 25.474 | 53.247  | 11.551 | 1.00 31.54 | 8 |
| 5863 | OWO WAT V 421 | 28.282 | 72.460  | 57.888 | 1.00 29.12 | 8 | 5905 | OWO WAT V 463 | 21.666 | 48.674  | 41.178 | 1.00 31.71 | 8 |
| 5864 | OWO WAT V 422 | 50.448 | 63.547  | 18.793 | 1.00 29.31 | 8 | 5906 | OWO WAT V 464 | 51.799 | 63.643  | 37.234 | 1.00 30.69 | 8 |
| 5865 | OWO WAT V 423 | 43.033 | 55.323  | 65.913 | 1.00 29.32 | 8 | 5907 | OWO WAT V 465 | 17.686 | 48.668  | 36.134 | 1.00 31.38 | 8 |
| 5866 | OWO WAT V 424 | 45.865 | 51.168  | 51.498 | 1.00 29.29 | 8 | 5908 | OWO WAT V 466 | 47.081 | 52.951  | 49.717 | 1.00 30.51 | 8 |
| 5867 | OWO WAT V 425 | 12.844 | 59.751  | 19.386 | 1.00 29.45 | 8 | 5909 | OWO WAT V 467 | 15.593 | 93.203  | 42.768 | 1.00 30.90 | 8 |
| 5868 | OWO WAT V 426 | -3.707 | 82.697  | 22.959 | 1.00 29.58 | 8 | 5910 | OWO WAT V 468 | 36.480 | 80.071  | 53.771 | 1.00 30.56 | 8 |
| 5869 | OWO WAT V 427 | 28.989 | 45.171  | 18.941 | 1.00 29.97 | 8 | 5911 | OWO WAT V 469 | 42.137 | 47.781  | 14.882 | 1.00 31.85 | 8 |
| 5870 | OWO WAT V 428 | 14.689 | 65.149  | 11.472 | 1.00 29.76 | 8 | 5912 | OWO WAT V 470 | 22.333 | 61.351  | 70.096 | 1.00 31.36 | 8 |
| 5871 | OWO WAT V 429 | 49.962 | 74.061  | 53.225 | 1.00 29.59 | 8 | 5913 | OWO WAT V 471 | 40.228 | 72.527  | 72.095 | 1.00 31.17 | 8 |
| 5872 | OWO WAT V 430 | 26.674 | 46.428  | 17.647 | 1.00 29.59 | 8 | 5914 | OWO WAT V 472 | 1.666  | 74.527  | 48.132 | 1.00 31.28 | 8 |
| 5873 | OWO WAT V 431 | 32.017 | 64.281  | 73.846 | 1.00 29.67 | 8 | 5915 | OWO WAT V 473 | 14.531 | 66.936  | 59.718 | 1.00 31.26 | 8 |
| 5874 | OWO WAT V 432 | -1.685 | 89.735  | 36.396 | 1.00 29.42 | 8 | 5916 | OWO WAT V 474 | 21.000 | 68.421  | 1.879  | 1.00 31.59 | 8 |
| 5875 | OWO WAT V 433 | 35.326 | 90.671  | 32.858 | 1.00 30.08 | 8 | 5917 | OWO WAT V 475 | 37.163 | 82.170  | 41.385 | 1.00 31.32 | 8 |
| 5876 | OWO WAT V 434 | -5.217 | 86.519  | 22.737 | 1.00 30.64 | 8 | 5918 | OWO WAT V 476 | 26.307 | 62.094  | 4.445  | 1.00 31.75 | 8 |
| 5877 | OWO WAT V 435 | 22.655 | 40.619  | 31.468 | 1.00 30.18 | 8 | 5919 | OWO WAT V 477 | 51.579 | 61.409  | 40.641 | 1.00 31.25 | 8 |
| 5878 | OWO WAT V 436 | 9.970  | 66.686  | 21.940 | 1.00 30.16 | 8 | 5920 | OWO WAT V 478 | 41.761 | 64.533  | 7.578  | 1.00 31.59 | 8 |
| 5879 | OWO WAT V 437 | 22.156 | 103.267 | 41.579 | 1.00 28.97 | 8 | 5921 | OWO WAT V 479 | -7.353 | 65.632  | 35.219 | 1.00 31.13 | 8 |
| 5880 | OWO WAT V 438 | 40.919 | 45.553  | 23.996 | 1.00 30.13 | 8 | 5922 | OWO WAT V 480 | 16.514 | 82.720  | 36.237 | 1.00 31.25 | 8 |
| 5881 | OWO WAT V 439 | 24.378 | 42.994  | 18.498 | 1.00 30.29 | 8 | 5923 | OWO WAT V 481 | 23.770 | 75.891  | 54.586 | 1.00 31.53 | 8 |
| 5882 | OWO WAT V 440 | 27.456 | 90.485  | 38.760 | 1.00 29.87 | 8 | 5924 | OWO WAT V 482 | 50.377 | 68.458  | 56.245 | 1.00 31.72 | 8 |
| 5883 | OWO WAT V 441 | 41.628 | 78.372  | 57.406 | 1.00 30.24 | 8 | 5925 | OWO WAT V 483 | 15.979 | 105.053 | 38.501 | 1.00 30.98 | 8 |
| 5884 | OWO WAT V 442 | 10.162 | 67.365  | 58.879 | 1.00 30.51 | 8 | 5926 | OWO WAT V 484 | 27.194 | 93.867  | 31.829 | 1.00 31.85 | 8 |
| 5885 | OWO WAT V 443 | 7.899  | 70.258  | 55.642 | 1.00 29.98 | 8 | 5927 | OWO WAT V 485 | 39.487 | 68.664  | 5.438  | 1.00 31.02 | 8 |
| 5886 | OWO WAT V 444 | 7.439  | 62.721  | 58.664 | 1.00 30.04 | 8 | 5928 | OWO WAT V 486 | 30.446 | 58.438  | 75.573 | 1.00 31.49 | 8 |
| 5887 | OWO WAT V 445 | 30.182 | 60.296  | 5.170  | 1.00 30.62 | 8 | 5929 | OWO WAT V 487 | -2.258 | 85.349  | 34.418 | 1.00 31.74 | 8 |
| 5888 | OWO WAT V 446 | 36.835 | 87.065  | 16.010 | 1.00 30.22 | 8 | 5930 | OWO WAT V 488 | 46.873 | 56.769  | 65.770 | 1.00 31.57 | 8 |
| 5889 | OWO WAT V 447 | 48.154 | 58.076  | 55.789 | 1.00 30.39 | 8 | 5931 | OWO WAT V 489 | 18.407 | 47.617  | 19.229 | 1.00 31.61 | 8 |
| 5890 | OWO WAT V 448 | 9.079  | 102.838 | 38.708 | 1.00 30.45 | 8 | 5932 | OWO WAT V 490 | 2.500  | 78.686  | 43.392 | 1.00 31.62 | 8 |
| 5891 | OWO WAT V 449 | 31.488 | 67.009  | 5.903  | 1.00 30.35 | 8 | 5933 | OWO WAT V 491 | 7.727  | 97.913  | 42.497 | 1.00 32.36 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 5934 | OWO WAT V 492 | -5.430 | 71.658  | 30.991 | 1.00 | 32.45 | 8 | 5976 | OWO WAT V 534 | 35.615 | 48.266  | 53.410 | 1.00 | 33.74 | 8 |
| 5935 | OWO WAT V 493 | 47.547 | 72.958  | 21.222 | 1.00 | 31.57 | 8 | 5977 | OWO WAT V 535 | 50.581 | 54.379  | 41.752 | 1.00 | 32.75 | 8 |
| 5936 | OWO WAT V 494 | 9.955  | 91.961  | 24.393 | 1.00 | 32.43 | 8 | 5978 | OWO WAT V 536 | 34.738 | 50.213  | 7.372  | 1.00 | 33.68 | 8 |
| 5937 | OWO WAT V 495 | 12.996 | 52.420  | 46.232 | 1.00 | 31.76 | 8 | 5979 | OWO WAT V 537 | 42.324 | 79.266  | 54.340 | 1.00 | 32.72 | 8 |
| 5938 | OWO WAT V 496 | 7.952  | 65.594  | 58.841 | 1.00 | 32.02 | 8 | 5980 | OWO WAT V 538 | 16.132 | 78.441  | 8.864  | 1.00 | 33.64 | 8 |
| 5939 | OWO WAT V 497 | 37.204 | 88.789  | 33.415 | 1.00 | 31.57 | 8 | 5981 | OWO WAT V 539 | 20.256 | 45.911  | 20.702 | 1.00 | 33.89 | 8 |
| 5940 | OWO WAT V 498 | 36.857 | 41.938  | 29.865 | 1.00 | 32.38 | 8 | 5982 | OWO WAT V 540 | 37.253 | 43.882  | 46.170 | 1.00 | 33.73 | 8 |
| 5941 | OWO WAT V 499 | 7.220  | 51.844  | 54.727 | 1.00 | 32.32 | 8 | 5983 | OWO WAT V 541 | 31.158 | 88.960  | 12.651 | 1.00 | 34.15 | 8 |
| 5942 | OWO WAT V 500 | 16.110 | 76.377  | 49.777 | 1.00 | 32.31 | 8 | 5984 | OWO WAT V 542 | 2.885  | 65.252  | 30.182 | 1.00 | 33.66 | 8 |
| 5943 | OWO WAT V 501 | 24.511 | 47.736  | 42.135 | 1.00 | 32.37 | 8 | 5985 | OWO WAT V 543 | 24.093 | 72.008  | 54.068 | 1.00 | 33.53 | 8 |
| 5944 | OWO WAT V 502 | 22.783 | 46.357  | 48.051 | 1.00 | 32.64 | 8 | 5986 | OWO WAT V 544 | -4.660 | 58.902  | 52.534 | 1.00 | 34.13 | 8 |
| 5945 | OWO WAT V 503 | 27.138 | 60.897  | 7.569  | 1.00 | 32.20 | 8 | 5987 | OWO WAT V 545 | 20.523 | 52.571  | 71.335 | 1.00 | 34.29 | 8 |
| 5946 | OWO WAT V 504 | 47.227 | 50.290  | 36.850 | 1.00 | 32.13 | 8 | 5988 | OWO WAT V 546 | 50.389 | 70.373  | 43.120 | 1.00 | 34.05 | 8 |
| 5947 | OWO WAT V 505 | 6.733  | 67.493  | 23.991 | 1.00 | 32.68 | 8 | 5989 | OWO WAT V 547 | -1.784 | 74.917  | 34.717 | 1.00 | 34.27 | 8 |
| 5948 | OWO WAT V 506 | 16.514 | 70.176  | 56.941 | 1.00 | 32.03 | 8 | 5990 | OWO WAT V 548 | 25.051 | 100.468 | 31.517 | 1.00 | 33.73 | 8 |
| 5949 | OWO WAT V 507 | 43.175 | 79.662  | 8.514  | 1.00 | 31.76 | 8 | 5991 | OWO WAT V 549 | 21.989 | 83.148  | 46.194 | 1.00 | 34.71 | 8 |
| 5950 | OWO WAT V 508 | -3.757 | 80.394  | 22.899 | 1.00 | 32.62 | 8 | 5992 | OWO WAT V 550 | 47.521 | 62.364  | 11.718 | 1.00 | 34.05 | 8 |
| 5951 | OWO WAT V 509 | 10.932 | 85.936  | 45.262 | 1.00 | 32.65 | 8 | 5993 | OWO WAT V 551 | 52.236 | 59.305  | 62.786 | 1.00 | 33.21 | 8 |
| 5952 | OWO WAT V 510 | 3.455  | 97.650  | 41.755 | 1.00 | 32.31 | 8 | 5994 | OWO WAT V 552 | 40.232 | 80.510  | 16.448 | 1.00 | 34.62 | 8 |
| 5953 | OWO WAT V 511 | 33.419 | 50.551  | 69.455 | 1.00 | 32.14 | 8 | 5995 | OWO WAT V 553 | 46.253 | 56.949  | 70.930 | 1.00 | 33.53 | 8 |
| 5954 | OWO WAT V 512 | 4.069  | 99.962  | 23.550 | 1.00 | 33.21 | 8 | 5996 | OWO WAT V 554 | 47.895 | 53.053  | 37.454 | 1.00 | 33.41 | 8 |
| 5955 | OWO WAT V 513 | -7.206 | 65.717  | 41.690 | 1.00 | 33.20 | 8 | 5997 | OWO WAT V 555 | 13.358 | 71.030  | 49.662 | 1.00 | 34.43 | 8 |
| 5956 | OWO WAT V 514 | 53.785 | 60.262  | 61.406 | 1.00 | 33.37 | 8 | 5998 | OWO WAT V 556 | -0.137 | 73.990  | 26.087 | 1.00 | 34.05 | 8 |
| 5957 | OWO WAT V 515 | 16.599 | 87.045  | 17.346 | 1.00 | 32.99 | 8 | 5999 | OWO WAT V 557 | 43.973 | 74.382  | 6.399  | 1.00 | 34.44 | 8 |
| 5958 | OWO WAT V 516 | 47.349 | 54.074  | 30.752 | 1.00 | 32.14 | 8 | 6000 | OWO WAT V 558 | 35.593 | 60.367  | 77.022 | 1.00 | 33.63 | 8 |
| 5959 | OWO WAT V 517 | 7.038  | 85.163  | 42.409 | 1.00 | 32.78 | 8 | 6001 | OWO WAT V 559 | 6.112  | 83.592  | 41.192 | 1.00 | 34.97 | 8 |
| 5960 | OWO WAT V 518 | 16.879 | 50.503  | 27.538 | 1.00 | 32.69 | 8 | 6002 | OWO WAT V 560 | 38.614 | 41.425  | 25.492 | 1.00 | 34.42 | 8 |
| 5961 | OWO WAT V 519 | 30.838 | 91.776  | 22.385 | 1.00 | 33.06 | 8 | 6003 | OWO WAT V 561 | 34.074 | 88.144  | 12.960 | 1.00 | 34.41 | 8 |
| 5962 | OWO WAT V 520 | 33.882 | 41.296  | 32.218 | 1.00 | 33.06 | 8 | 6004 | OWO WAT V 562 | 40.114 | 63.213  | 5.786  | 1.00 | 34.56 | 8 |
| 5963 | OWO WAT V 521 | 53.502 | 60.512  | 23.358 | 1.00 | 32.27 | 8 | 6005 | OWO WAT V 563 | -0.202 | 64.215  | 60.019 | 1.00 | 34.60 | 8 |
| 5964 | OWO WAT V 522 | 41.841 | 73.003  | 34.316 | 1.00 | 33.63 | 8 | 6006 | OWO WAT V 564 | 4.614  | 92.264  | 20.329 | 1.00 | 33.82 | 8 |
| 5965 | OWO WAT V 523 | 18.807 | 69.394  | 5.371  | 1.00 | 32.65 | 8 | 6007 | OWO WAT V 565 | 15.212 | 50.738  | 32.687 | 1.00 | 34.54 | 8 |
| 5966 | OWO WAT V 524 | 0.567  | 102.365 | 27.670 | 1.00 | 32.87 | 8 | 6008 | OWO WAT V 566 | 13.018 | 70.753  | 53.378 | 1.00 | 35.00 | 8 |
| 5967 | OWO WAT V 525 | 28.899 | 48.822  | 64.451 | 1.00 | 32.62 | 8 | 6009 | OWO WAT V 567 | 37.836 | 57.700  | 75.968 | 1.00 | 33.91 | 8 |
| 5968 | OWO WAT V 526 | 42.766 | 46.627  | 21.339 | 1.00 | 33.04 | 8 | 6010 | OWO WAT V 568 | 18.054 | 71.354  | 7.047  | 1.00 | 34.28 | 8 |
| 5969 | OWO WAT V 527 | 18.159 | 66.472  | 60.034 | 1.00 | 33.02 | 8 | 6011 | OWO WAT V 569 | 20.435 | 57.091  | 12.782 | 1.00 | 34.06 | 8 |
| 5970 | OWO WAT V 528 | 22.385 | 49.518  | 59.427 | 1.00 | 33.48 | 8 | 6012 | OWO WAT V 570 | -1.113 | 72.836  | 30.802 | 1.00 | 34.18 | 8 |
| 5971 | OWO WAT V 529 | 14.542 | 53.899  | 35.438 | 1.00 | 32.40 | 8 | 6013 | OWO WAT V 571 | 45.394 | 47.985  | 15.576 | 1.00 | 34.25 | 8 |
| 5972 | OWO WAT V 530 | 0.923  | 81.260  | 18.821 | 1.00 | 33.19 | 8 | 6014 | OWO WAT V 572 | 18.083 | 105.524 | 25.739 | 1.00 | 35.26 | 8 |
| 5973 | OWO WAT V 531 | 35.980 | 91.602  | 25.073 | 1.00 | 32.89 | 8 | 6015 | OWO WAT V 573 | 42.363 | 51.035  | 61.868 | 1.00 | 34.64 | 8 |
| 5974 | OWO WAT V 532 | 40.667 | 67.024  | 71.313 | 1.00 | 32.79 | 8 | 6016 | OWO WAT V 574 | 3.332  | 65.717  | 27.045 | 1.00 | 35.54 | 8 |
| 5975 | OWO WAT V 533 | 8.626  | 61.294  | 60.713 | 1.00 | 32.69 | 8 | 6017 | OWO WAT V 575 | 0.099  | 70.672  | 51.291 | 1.00 | 34.72 | 8 |





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|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| 6102 | OWO | WAT | V | 660 | 23.932 | 65.246  | 70.893 | 1.00 | 37.09 | 8 | 6144 | OWO | WAT | V | 702 | 36.514 | 82.654  | 34.129 | 1.00 | 38.10 | 8 |
| 6103 | OWO | WAT | V | 661 | 0.664  | 53.286  | 53.271 | 1.00 | 38.36 | 8 | 6145 | OWO | WAT | V | 703 | 43.559 | 50.161  | 59.718 | 1.00 | 39.15 | 8 |
| 6104 | OWO | WAT | V | 662 | 40.187 | 84.151  | 18.538 | 1.00 | 38.05 | 8 | 6146 | OWO | WAT | V | 704 | 41.881 | 70.064  | 7.497  | 1.00 | 39.49 | 8 |
| 6105 | OWO | WAT | V | 663 | 44.129 | 77.826  | 7.095  | 1.00 | 38.36 | 8 | 6147 | OWO | WAT | V | 705 | 12.039 | 106.892 | 30.442 | 1.00 | 39.69 | 8 |
| 6106 | OWO | WAT | V | 664 | 5.654  | 103.176 | 36.651 | 1.00 | 38.12 | 8 | 6148 | OWO | WAT | V | 706 | 25.673 | 81.581  | 52.252 | 1.00 | 39.17 | 8 |
| 6107 | OWO | WAT | V | 665 | -2.551 | 55.092  | 37.581 | 1.00 | 39.63 | 8 | 6149 | OWO | WAT | V | 707 | 21.077 | 93.052  | 26.181 | 1.00 | 40.35 | 8 |
| 6108 | OWO | WAT | V | 666 | 48.102 | 56.702  | 13.267 | 1.00 | 37.64 | 8 | 6150 | OWO | WAT | V | 708 | 46.855 | 74.915  | 26.181 | 1.00 | 40.35 | 8 |
| 6109 | OWO | WAT | V | 667 | 27.824 | 90.475  | 15.555 | 1.00 | 36.41 | 8 | 6151 | OWO | WAT | V | 709 | 28.621 | 62.328  | 5.470  | 1.00 | 38.56 | 8 |
| 6110 | OWO | WAT | V | 668 | 38.699 | 49.812  | 63.112 | 1.00 | 37.80 | 8 | 6152 | OWO | WAT | V | 710 | -3.607 | 57.742  | 54.506 | 1.00 | 38.82 | 8 |
| 6111 | OWO | WAT | V | 669 | -2.199 | 54.401  | 53.588 | 1.00 | 39.21 | 8 | 6153 | OWO | WAT | V | 711 | 25.913 | 41.714  | 29.843 | 1.00 | 38.94 | 8 |
| 6112 | OWO | WAT | V | 670 | 19.006 | 53.240  | 47.228 | 1.00 | 38.93 | 8 | 6154 | OWO | WAT | V | 712 | 21.385 | 95.763  | 42.160 | 1.00 | 39.85 | 8 |
| 6113 | OWO | WAT | V | 671 | 46.897 | 48.817  | 19.829 | 1.00 | 39.11 | 8 | 6155 | OWO | WAT | V | 713 | 39.666 | 46.565  | 56.093 | 1.00 | 40.16 | 8 |
| 6114 | OWO | WAT | V | 672 | 42.301 | 48.935  | 12.664 | 1.00 | 37.43 | 8 | 6156 | OWO | WAT | V | 714 | 33.043 | 47.398  | 12.747 | 1.00 | 38.56 | 8 |
| 6115 | OWO | WAT | V | 673 | 16.098 | 53.972  | 53.322 | 1.00 | 38.55 | 8 | 6157 | OWO | WAT | V | 715 | 3.335  | 48.480  | 47.523 | 1.00 | 40.24 | 8 |
| 6116 | OWO | WAT | V | 674 | 16.992 | 66.360  | 61.965 | 1.00 | 40.47 | 8 | 6158 | OWO | WAT | V | 716 | -5.954 | 59.355  | 43.289 | 1.00 | 39.30 | 8 |
| 6117 | OWO | WAT | V | 675 | 17.396 | 84.259  | 14.592 | 1.00 | 37.45 | 8 | 6159 | OWO | WAT | V | 717 | -2.633 | 70.380  | 52.100 | 1.00 | 39.49 | 8 |
| 6118 | OWO | WAT | V | 676 | 48.023 | 70.300  | 38.414 | 1.00 | 38.28 | 8 | 6160 | OWO | WAT | V | 718 | 14.943 | 51.881  | 28.927 | 1.00 | 41.17 | 8 |
| 6119 | OWO | WAT | V | 677 | 21.061 | 60.355  | 72.008 | 1.00 | 38.68 | 8 | 6161 | OWO | WAT | V | 719 | 30.665 | 55.789  | 76.270 | 1.00 | 36.29 | 8 |
| 6120 | OWO | WAT | V | 678 | 25.412 | 45.777  | 15.102 | 1.00 | 40.05 | 8 | 6162 | OWO | WAT | V | 720 | 38.153 | 41.243  | 44.336 | 1.00 | 39.61 | 8 |
| 6121 | OWO | WAT | V | 679 | 43.705 | 73.272  | 1.624  | 1.00 | 38.78 | 8 | 6163 | OWO | WAT | V | 721 | 42.857 | 72.924  | 4.760  | 1.00 | 39.33 | 8 |
| 6122 | OWO | WAT | V | 680 | 17.379 | 67.334  | 7.173  | 1.00 | 38.88 | 8 | 6164 | OWO | WAT | V | 722 | 42.983 | 45.506  | 30.086 | 1.00 | 39.35 | 8 |
| 6123 | OWO | WAT | V | 681 | 19.500 | 72.583  | 5.113  | 1.00 | 41.12 | 8 | 6165 | OWO | WAT | V | 723 | 8.541  | 68.671  | 15.477 | 1.00 | 40.10 | 8 |
| 6124 | OWO | WAT | V | 682 | 27.135 | 53.269  | 75.096 | 1.00 | 38.74 | 8 | 6166 | OWO | WAT | V | 724 | 3.357  | 68.745  | 24.682 | 1.00 | 39.21 | 8 |
| 6125 | OWO | WAT | V | 683 | 43.871 | 76.670  | 2.397  | 1.00 | 38.42 | 8 | 6167 | OWO | WAT | V | 725 | 32.096 | 74.899  | 2.155  | 1.00 | 38.68 | 8 |
| 6126 | OWO | WAT | V | 684 | 32.690 | 47.277  | 60.342 | 1.00 | 38.23 | 8 | 6168 | OWO | WAT | V | 726 | -3.316 | 99.677  | 31.930 | 1.00 | 40.29 | 8 |
| 6127 | OWO | WAT | V | 685 | 38.889 | 50.643  | 67.387 | 1.00 | 38.05 | 8 | 6169 | OWO | WAT | V | 727 | 33.290 | 44.355  | 45.552 | 1.00 | 39.94 | 8 |
| 6128 | OWO | WAT | V | 686 | 15.848 | 75.816  | 7.403  | 1.00 | 37.86 | 8 | 6170 | OWO | WAT | V | 728 | 50.677 | 69.314  | 25.213 | 1.00 | 38.89 | 8 |
| 6129 | OWO | WAT | V | 687 | 25.036 | 96.149  | 30.003 | 1.00 | 38.02 | 8 | 6171 | OWO | WAT | V | 729 | 35.441 | 42.395  | 37.048 | 1.00 | 39.29 | 8 |
| 6130 | OWO | WAT | V | 688 | 44.120 | 49.147  | 54.661 | 1.00 | 39.21 | 8 | 6172 | OWO | WAT | V | 730 | 8.363  | 53.922  | 35.516 | 1.00 | 38.32 | 8 |
| 6131 | OWO | WAT | V | 689 | 31.793 | 51.208  | 10.937 | 1.00 | 39.53 | 8 | 6173 | OWO | WAT | V | 731 | -1.713 | 91.588  | 39.071 | 1.00 | 40.09 | 8 |
| 6132 | OWO | WAT | V | 690 | 9.476  | 96.492  | 43.783 | 1.00 | 37.31 | 8 | 6174 | OWO | WAT | V | 732 | 22.068 | 82.950  | 49.452 | 1.00 | 38.86 | 8 |
| 6133 | OWO | WAT | V | 691 | 8.821  | 88.129  | 44.638 | 1.00 | 39.95 | 8 | 6175 | OWO | WAT | V | 733 | -1.449 | 89.011  | 21.652 | 1.00 | 39.99 | 8 |
| 6134 | OWO | WAT | V | 692 | 8.003  | 80.636  | 43.644 | 1.00 | 37.70 | 8 | 6176 | OWO | WAT | V | 734 | 37.354 | 59.035  | 5.289  | 1.00 | 40.90 | 8 |
| 6135 | OWO | WAT | V | 693 | 14.834 | 83.314  | 13.883 | 1.00 | 39.80 | 8 | 6177 | OWO | WAT | V | 735 | 20.992 | 87.687  | 45.698 | 1.00 | 40.19 | 8 |
| 6136 | OWO | WAT | V | 694 | 21.370 | 44.389  | 41.265 | 1.00 | 39.75 | 8 | 6178 | OWO | WAT | V | 736 | 46.650 | 76.726  | 54.492 | 1.00 | 40.47 | 8 |
| 6137 | OWO | WAT | V | 695 | 25.208 | 85.122  | 7.995  | 1.00 | 38.90 | 8 | 6179 | OWO | WAT | V | 737 | 7.370  | 47.777  | 49.173 | 1.00 | 41.37 | 8 |
| 6138 | OWO | WAT | V | 696 | 34.431 | 64.498  | 5.882  | 1.00 | 37.43 | 8 | 6180 | OWO | WAT | V | 738 | 14.279 | 71.404  | 55.742 | 1.00 | 39.06 | 8 |
| 6139 | OWO | WAT | V | 697 | 46.857 | 48.623  | 44.260 | 1.00 | 38.67 | 8 | 6181 | OWO | WAT | V | 739 | 13.276 | 62.067  | 63.468 | 1.00 | 38.95 | 8 |
| 6140 | OWO | WAT | V | 698 | 48.394 | 49.074  | 31.806 | 1.00 | 38.40 | 8 | 6182 | OWO | WAT | V | 740 | 47.469 | 55.262  | 33.788 | 1.00 | 41.14 | 8 |
| 6141 | OWO | WAT | V | 699 | 6.330  | 71.875  | 18.323 | 1.00 | 39.24 | 8 | 6183 | OWO | WAT | V | 741 | 35.182 | 72.963  | 73.409 | 1.00 | 38.69 | 8 |
| 6142 | OWO | WAT | V | 700 | 3.567  | 68.493  | 56.513 | 1.00 | 39.03 | 8 | 6184 | OWO | WAT | V | 742 | 28.993 | 42.749  | 41.796 | 1.00 | 40.22 | 8 |
| 6143 | OWO | WAT | V | 701 | 19.531 | 67.580  | 61.273 | 1.00 | 38.68 | 8 | 6185 | OWO | WAT | V | 743 | 12.430 | 51.804  | 37.400 | 1.00 | 39.68 | 8 |

|      |               |        |         |        |            |   |      |               |        |         |        |            |   |
|------|---------------|--------|---------|--------|------------|---|------|---------------|--------|---------|--------|------------|---|
| 6186 | OWO WAT V 744 | 5.325  | 85.408  | 18.950 | 1.00 41.26 | 8 | 6228 | OWO WAT V 786 | 19.476 | 44.845  | 23.558 | 1.00 42.02 | 8 |
| 6187 | OWO WAT V 745 | 41.721 | 66.169  | 73.677 | 1.00 39.43 | 8 | 6229 | OWO WAT V 787 | 21.294 | 88.109  | 18.755 | 1.00 42.02 | 8 |
| 6188 | OWO WAT V 746 | 16.983 | 83.519  | 10.040 | 1.00 40.83 | 8 | 6230 | OWO WAT V 788 | 46.461 | 57.071  | 56.124 | 1.00 41.88 | 8 |
| 6189 | OWO WAT V 747 | -3.245 | 67.552  | 51.568 | 1.00 41.14 | 8 | 6231 | OWO WAT V 789 | 52.975 | 62.124  | 50.393 | 1.00 41.59 | 8 |
| 6190 | OWO WAT V 748 | 18.547 | 72.699  | 54.390 | 1.00 40.80 | 8 | 6232 | OWO WAT V 790 | 8.480  | 108.235 | 24.221 | 1.00 42.16 | 8 |
| 6191 | OWO WAT V 749 | 50.952 | 65.503  | 10.665 | 1.00 39.71 | 8 | 6233 | OWO WAT V 791 | 18.517 | 78.200  | 51.474 | 1.00 42.31 | 8 |
| 6192 | OWO WAT V 750 | 6.873  | 59.618  | 31.097 | 1.00 40.61 | 8 | 6234 | OWO WAT V 792 | -5.150 | 51.726  | 49.471 | 1.00 40.85 | 8 |
| 6193 | OWO WAT V 751 | 44.643 | 72.249  | 41.540 | 1.00 40.21 | 8 | 6235 | OWO WAT V 793 | 36.849 | 55.447  | 72.633 | 1.00 42.13 | 8 |
| 6194 | OWO WAT V 752 | 10.333 | 59.620  | 21.158 | 1.00 40.03 | 8 | 6236 | OWO WAT V 794 | 37.563 | 79.694  | 42.494 | 1.00 41.67 | 8 |
| 6195 | OWO WAT V 753 | 25.342 | 99.843  | 20.985 | 1.00 40.88 | 8 | 6237 | OWO WAT V 795 | 18.818 | 84.285  | 16.222 | 1.00 43.03 | 8 |
| 6196 | OWO WAT V 754 | 13.886 | 67.341  | 51.913 | 1.00 41.40 | 8 | 6238 | OWO WAT V 796 | 36.451 | 82.759  | 13.933 | 1.00 41.71 | 8 |
| 6197 | OWO WAT V 755 | 20.669 | 50.466  | 56.076 | 1.00 40.93 | 8 | 6239 | OWO WAT V 797 | 22.906 | 51.457  | 67.808 | 1.00 41.33 | 8 |
| 6198 | OWO WAT V 756 | 16.062 | 51.352  | 42.439 | 0.00 41.08 | 8 | 6240 | OWO WAT V 798 | 1.528  | 102.171 | 36.053 | 1.00 41.41 | 8 |
| 6199 | OWO WAT V 757 | -2.323 | 91.095  | 34.519 | 1.00 40.69 | 8 | 6241 | OWO WAT V 799 | 36.684 | 45.294  | 51.188 | 1.00 42.88 | 8 |
| 6200 | OWO WAT V 758 | 3.987  | 63.229  | 29.353 | 1.00 41.53 | 8 | 6242 | OWO WAT V 800 | 14.017 | 67.414  | 9.706  | 1.00 41.87 | 8 |
| 6201 | OWO WAT V 759 | 20.694 | 99.900  | 18.786 | 1.00 39.84 | 8 | 6243 | OWO WAT V 801 | 47.832 | 66.788  | 18.650 | 1.00 43.94 | 8 |
| 6202 | OWO WAT V 760 | 21.098 | 72.115  | 58.710 | 1.00 40.04 | 8 | 6244 | OWO WAT V 802 | 34.436 | 88.324  | 36.102 | 1.00 43.03 | 8 |
| 6203 | OWO WAT V 761 | 39.451 | 41.349  | 13.513 | 1.00 40.57 | 8 | 6245 | OWO WAT V 803 | 24.260 | 67.815  | 69.741 | 1.00 42.57 | 8 |
| 6204 | OWO WAT V 762 | 3.185  | 80.792  | 42.000 | 1.00 41.27 | 8 | 6246 | OWO WAT V 804 | 13.129 | 74.685  | 52.293 | 1.00 42.14 | 8 |
| 6205 | OWO WAT V 763 | 15.866 | 68.494  | 52.407 | 1.00 40.90 | 8 | 6247 | OWO WAT V 805 | 16.572 | 61.433  | 12.722 | 1.00 41.61 | 8 |
| 6206 | OWO WAT V 764 | 42.027 | 79.686  | 47.257 | 1.00 40.14 | 8 | 6248 | OWO WAT V 806 | 46.827 | 51.429  | 47.524 | 1.00 42.73 | 8 |
| 6207 | OWO WAT V 765 | 41.063 | 55.022  | 68.081 | 1.00 42.98 | 8 | 6249 | OWO WAT V 807 | 26.546 | 48.730  | 71.404 | 1.00 42.47 | 8 |
| 6208 | OWO WAT V 766 | 15.728 | 85.261  | 16.175 | 1.00 42.08 | 8 | 6250 | OWO WAT V 808 | 33.308 | 76.572  | 61.813 | 1.00 42.82 | 8 |
| 6209 | OWO WAT V 767 | -8.665 | 63.541  | 41.234 | 1.00 40.98 | 8 | 6251 | OWO WAT V 809 | 16.314 | 98.564  | 17.363 | 1.00 42.43 | 8 |
| 6210 | OWO WAT V 768 | 28.828 | 85.580  | 44.440 | 1.00 40.75 | 8 | 6252 | OWO WAT V 810 | 47.038 | 73.620  | 61.642 | 1.00 43.62 | 8 |
| 6211 | OWO WAT V 769 | 46.504 | 46.346  | 43.773 | 1.00 40.98 | 8 | 6253 | OWO WAT V 811 | 23.301 | 74.541  | 1.386  | 1.00 44.52 | 8 |
| 6212 | OWO WAT V 770 | 52.964 | 61.429  | 54.373 | 1.00 41.49 | 8 | 6254 | OWO WAT V 812 | 23.719 | 88.481  | 37.683 | 1.00 40.46 | 8 |
| 6213 | OWO WAT V 771 | 25.001 | 95.005  | 39.507 | 1.00 41.35 | 8 | 6255 | OWO WAT V 813 | 31.440 | 60.185  | 76.751 | 1.00 43.11 | 8 |
| 6214 | OWO WAT V 772 | 4.818  | 62.633  | 59.449 | 1.00 41.54 | 8 | 6256 | OWO WAT V 814 | 16.573 | 101.550 | 19.316 | 1.00 43.14 | 8 |
| 6215 | OWO WAT V 773 | 18.916 | 60.160  | 66.080 | 1.00 41.09 | 8 | 6257 | OWO WAT V 815 | 4.201  | 55.069  | 57.571 | 1.00 42.80 | 8 |
| 6216 | OWO WAT V 774 | 27.033 | 88.841  | 12.019 | 1.00 41.39 | 8 | 6258 | OWO WAT V 816 | -5.755 | 72.609  | 47.268 | 1.00 41.92 | 8 |
| 6217 | OWO WAT V 775 | 13.803 | 67.385  | 57.044 | 1.00 41.01 | 8 | 6259 | OWO WAT V 817 | 23.802 | 106.033 | 28.040 | 1.00 42.13 | 8 |
| 6218 | OWO WAT V 776 | 11.356 | 101.651 | 18.715 | 1.00 42.40 | 8 | 6260 | OWO WAT V 818 | 28.580 | 91.427  | 35.569 | 1.00 44.77 | 8 |
| 6219 | OWO WAT V 777 | 50.379 | 57.839  | 57.286 | 1.00 38.80 | 8 | 6261 | OWO WAT V 819 | -6.927 | 74.495  | 44.783 | 1.00 42.39 | 8 |
| 6220 | OWO WAT V 778 | 9.739  | 81.288  | 44.991 | 1.00 38.14 | 8 | 6262 | OWO WAT V 820 | 42.898 | 80.745  | 21.282 | 1.00 42.72 | 8 |
| 6221 | OWO WAT V 779 | 26.770 | 45.470  | 14.155 | 1.00 39.31 | 8 | 6263 | OWO WAT V 821 | 44.594 | 48.996  | 19.414 | 1.00 42.65 | 8 |
| 6222 | OWO WAT V 780 | 51.219 | 61.900  | 12.424 | 1.00 42.17 | 8 | 6264 | OWO WAT V 822 | 22.357 | 66.608  | 68.417 | 1.00 43.63 | 8 |
| 6223 | OWO WAT V 781 | 44.665 | 53.194  | 62.632 | 1.00 40.09 | 8 | 6265 | OWO WAT V 823 | 25.576 | 50.604  | 10.991 | 1.00 43.85 | 8 |
| 6224 | OWO WAT V 782 | -4.332 | 57.891  | 45.992 | 1.00 43.38 | 8 | 6266 | OWO WAT V 824 | 47.220 | 77.741  | 25.726 | 1.00 44.91 | 8 |
| 6225 | OWO WAT V 783 | 54.313 | 63.995  | 27.513 | 1.00 40.34 | 8 | 6267 | OWO WAT V 825 | 16.600 | 55.517  | 47.156 | 1.00 44.33 | 8 |
| 6226 | OWO WAT V 784 | 26.835 | 56.319  | 8.446  | 1.00 41.42 | 8 | 6268 | OWO WAT V 826 | 1.892  | 50.074  | 39.116 | 1.00 42.83 | 8 |
| 6227 | OWO WAT V 785 | 53.198 | 59.584  | 25.852 | 1.00 42.12 | 8 | 6269 | OWO WAT V 827 | 24.440 | 89.039  | 35.388 | 1.00 43.51 | 8 |

|      |     |     |   |     |        |         |        |      |       |   |      |     |     |   |     |        |         |        |      |       |   |
|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| 6270 | OWO | WAT | V | 828 | 21.480 | 53.418  | 43.918 | 1.00 | 43.38 | 8 | 6312 | OWO | WAT | V | 870 | 46.779 | 45.863  | 33.183 | 1.00 | 38.06 | 8 |
| 6271 | OWO | WAT | V | 829 | 14.604 | 82.502  | 11.170 | 1.00 | 41.84 | 8 | 6313 | OWO | WAT | V | 871 | 28.449 | 47.238  | 49.410 | 1.00 | 44.98 | 8 |
| 6272 | OWO | WAT | V | 830 | 14.875 | 62.765  | 14.779 | 1.00 | 42.12 | 8 | 6314 | OWO | WAT | V | 872 | 31.691 | 90.618  | 16.034 | 1.00 | 45.59 | 8 |
| 6273 | OWO | WAT | V | 831 | 3.701  | 80.451  | 16.127 | 1.00 | 43.54 | 8 | 6315 | OWO | WAT | V | 873 | 45.269 | 73.271  | 25.041 | 1.00 | 46.87 | 8 |
| 6274 | OWO | WAT | V | 832 | 48.724 | 69.957  | 34.245 | 1.00 | 43.72 | 8 | 6316 | OWO | WAT | V | 874 | 18.096 | 50.245  | 53.261 | 1.00 | 45.09 | 8 |
| 6275 | OWO | WAT | V | 833 | 33.297 | 59.385  | 78.143 | 1.00 | 45.08 | 8 | 6317 | OWO | WAT | V | 875 | -5.062 | 64.679  | 39.520 | 1.00 | 44.00 | 8 |
| 6276 | OWO | WAT | V | 834 | 17.544 | 53.593  | 51.513 | 1.00 | 46.32 | 8 | 6318 | OWO | WAT | V | 876 | 17.006 | 54.092  | 49.423 | 1.00 | 46.50 | 8 |
| 6277 | OWO | WAT | V | 835 | 12.009 | 85.638  | 47.505 | 1.00 | 44.72 | 8 | 6319 | OWO | WAT | V | 877 | 39.580 | 64.107  | 77.580 | 1.00 | 45.16 | 8 |
| 6278 | OWO | WAT | V | 836 | 12.936 | 54.854  | 19.146 | 1.00 | 42.89 | 8 | 6320 | OWO | WAT | V | 878 | 16.405 | 56.330  | 66.595 | 1.00 | 44.67 | 8 |
| 6279 | OWO | WAT | V | 837 | 24.005 | 43.446  | 16.058 | 1.00 | 42.88 | 8 | 6321 | OWO | WAT | V | 879 | 28.253 | 74.829  | 0.308  | 1.00 | 44.14 | 8 |
| 6280 | OWO | WAT | V | 838 | 2.563  | 57.015  | 61.406 | 1.00 | 42.80 | 8 | 6322 | OWO | WAT | V | 880 | 26.165 | 96.027  | 33.730 | 1.00 | 45.73 | 8 |
| 6281 | OWO | WAT | V | 839 | 17.292 | 81.361  | 47.327 | 1.00 | 43.05 | 8 | 6323 | OWO | WAT | V | 881 | 25.024 | 94.673  | 31.684 | 1.00 | 45.30 | 8 |
| 6282 | OWO | WAT | V | 840 | 26.973 | 97.353  | 24.292 | 1.00 | 42.44 | 8 | 6324 | OWO | WAT | V | 882 | 6.382  | 101.590 | 23.078 | 1.00 | 45.88 | 8 |
| 6283 | OWO | WAT | V | 841 | 24.520 | 83.741  | 45.252 | 1.00 | 44.48 | 8 | 6325 | OWO | WAT | V | 883 | 20.784 | 106.032 | 25.469 | 1.00 | 44.92 | 8 |
| 6284 | OWO | WAT | V | 842 | 40.943 | 89.452  | 22.148 | 1.00 | 43.11 | 8 | 6326 | OWO | WAT | V | 884 | 15.678 | 70.001  | 59.741 | 1.00 | 47.72 | 8 |
| 6285 | OWO | WAT | V | 843 | 17.748 | 68.046  | 54.218 | 1.00 | 43.50 | 8 | 6327 | OWO | WAT | V | 885 | 43.426 | 78.175  | 61.043 | 1.00 | 46.23 | 8 |
| 6286 | OWO | WAT | V | 844 | 53.072 | 63.513  | 23.413 | 1.00 | 44.03 | 8 | 6328 | OWO | WAT | V | 886 | 10.651 | 50.358  | 43.666 | 1.00 | 45.79 | 8 |
| 6287 | OWO | WAT | V | 845 | -1.018 | 97.468  | 34.805 | 1.00 | 44.47 | 8 | 6329 | OWO | WAT | V | 887 | 0.918  | 49.811  | 54.685 | 1.00 | 45.38 | 8 |
| 6288 | OWO | WAT | V | 846 | 14.885 | 69.989  | 10.290 | 1.00 | 44.92 | 8 | 6330 | OWO | WAT | V | 888 | 24.371 | 106.460 | 30.607 | 1.00 | 46.20 | 8 |
| 6289 | OWO | WAT | V | 847 | 15.800 | 50.802  | 20.677 | 1.00 | 46.01 | 8 | 6331 | OWO | WAT | V | 889 | 7.425  | 93.590  | 16.782 | 1.00 | 45.79 | 8 |
| 6290 | OWO | WAT | V | 848 | 25.982 | 102.118 | 29.899 | 1.00 | 44.94 | 8 | 6332 | OWO | WAT | V | 890 | 20.314 | 66.093  | 66.469 | 1.00 | 48.35 | 8 |
| 6291 | OWO | WAT | V | 849 | 0.247  | 52.205  | 55.53  |      |       |   |      |     |     |   |     |        |         |        |      |       |   |



|      |               |        |         |        |            |   |      |               |        |         |        |            |   |
|------|---------------|--------|---------|--------|------------|---|------|---------------|--------|---------|--------|------------|---|
| 6438 | OWO WAT W 96  | 21.436 | 52.799  | 12.475 | 1.00 60.39 | 8 | 6480 | OWO WAT W 138 | 38.033 | 48.935  | 8.928  | 1.00 56.21 | 8 |
| 6439 | OWO WAT W 97  | 24.857 | 50.122  | 68.228 | 1.00 61.97 | 8 | 6481 | OWO WAT W 139 | 22.720 | 48.167  | 43.406 | 1.00 43.05 | 8 |
| 6440 | OWO WAT W 98  | 53.436 | 60.942  | 47.809 | 1.00 59.88 | 8 | 6482 | OWO WAT W 140 | 16.160 | 51.440  | 42.398 | 1.00 42.33 | 8 |
| 6441 | OWO WAT W 99  | 26.545 | 99.863  | 28.613 | 1.00 66.13 | 8 | 6483 | OWO WAT W 141 | 51.286 | 65.520  | 30.747 | 0.00 58.93 | 8 |
| 6442 | OWO WAT W 100 | 28.187 | 94.100  | 34.809 | 1.00 47.55 | 8 | 6484 | OWO WAT W 142 | 22.870 | 83.783  | -0.279 | 1.00 39.91 | 8 |
| 6443 | OWO WAT W 101 | 46.501 | 68.477  | 9.327  | 1.00 62.49 | 8 | 6485 | OWO WAT W 143 | 23.492 | 85.411  | 14.742 | 1.00 45.55 | 8 |
| 6444 | OWO WAT W 102 | 41.335 | 80.622  | 32.546 | 1.00 56.46 | 8 | 6486 | OWO WAT W 144 | 30.609 | 38.135  | 34.869 | 1.00 53.23 | 8 |
| 6445 | OWO WAT W 103 | 49.090 | 47.019  | 29.937 | 1.00 51.60 | 8 | 6487 | OWO WAT W 145 | 51.546 | 53.971  | 47.725 | 0.00 54.90 | 8 |
| 6446 | OWO WAT W 104 | 29.677 | 70.505  | 75.480 | 1.00 55.52 | 8 | 6488 | OWO WAT W 146 | 37.344 | 40.493  | 33.234 | 1.00 46.02 | 8 |
| 6447 | OWO WAT W 105 | 10.580 | 70.552  | 56.020 | 1.00 45.60 | 8 | 6489 | OWO WAT W 147 | 35.805 | 47.572  | 62.190 | 1.00 53.24 | 8 |
| 6448 | OWO WAT W 106 | -5.437 | 61.460  | 36.195 | 1.00 49.58 | 8 | 6490 | OWO WAT W 148 | 32.439 | 62.293  | 76.111 | 1.00 52.51 | 8 |
| 6449 | OWO WAT W 107 | 41.636 | 42.378  | 28.372 | 1.00 47.73 | 8 | 6491 | OWO WAT W 149 | 24.077 | 90.751  | 37.673 | 1.00 48.00 | 8 |
| 6450 | OWO WAT W 108 | 48.134 | 51.375  | 29.584 | 1.00 53.67 | 8 | 6492 | OWO WAT W 150 | 20.655 | 50.869  | 68.464 | 1.00 51.34 | 8 |
| 6451 | OWO WAT W 109 | 20.029 | 46.534  | 41.141 | 1.00 45.69 | 8 | 6493 | OWO WAT W 151 | 42.359 | 76.800  | 31.368 | 1.00 54.68 | 8 |
| 6452 | OWO WAT W 110 | 39.076 | 61.857  | 77.827 | 1.00 61.24 | 8 | 6494 | OWO WAT W 152 | 40.991 | 84.869  | 28.522 | 1.00 51.94 | 8 |
| 6453 | OWO WAT W 111 | 40.140 | 79.602  | 28.296 | 1.00 58.08 | 8 | 6495 | OWO WAT W 153 | -3.448 | 59.486  | 34.298 | 1.00 60.14 | 8 |
| 6454 | OWO WAT W 112 | 24.479 | 41.686  | 38.003 | 1.00 48.71 | 8 | 6496 | OWO WAT W 154 | 24.275 | 50.044  | 65.629 | 1.00 48.99 | 8 |
| 6455 | OWO WAT W 113 | 18.748 | 86.522  | 18.736 | 1.00 54.95 | 8 | 6497 | OWO WAT W 155 | 24.898 | 47.635  | 57.042 | 1.00 50.00 | 8 |
| 6456 | OWO WAT W 114 | 26.670 | 86.155  | 43.878 | 1.00 45.83 | 8 | 6498 | OWO WAT W 156 | 46.911 | 73.376  | 32.086 | 1.00 65.97 | 8 |
| 6457 | OWO WAT W 115 | 34.014 | 44.101  | 58.947 | 1.00 55.80 | 8 | 6499 | OWO WAT W 157 | 12.448 | 63.643  | 14.806 | 1.00 50.68 | 8 |
| 6458 | OWO WAT W 116 | 44.085 | 44.358  | 32.579 | 1.00 66.42 | 8 | 6500 | OWO WAT W 158 | 17.367 | 83.516  | 7.750  | 1.00 59.03 | 8 |
| 6459 | OWO WAT W 117 | 2.549  | 102.526 | 41.260 | 1.00 56.37 | 8 | 6501 | OWO WAT W 159 | 38.537 | 87.429  | 19.244 | 1.00 48.05 | 8 |
| 6460 | OWO WAT W 118 | 10.042 | 59.115  | 64.251 | 1.00 53.53 | 8 | 6502 | OWO WAT W 160 | 49.397 | 68.482  | 30.753 | 0.00 47.12 | 8 |
| 6461 | OWO WAT W 119 | 52.498 | 59.271  | 37.676 | 1.00 46.44 | 8 | 6503 | OWO WAT W 161 | 52.562 | 62.737  | 30.460 | 0.00 55.04 | 8 |
| 6462 | OWO WAT W 120 | 49.412 | 68.479  | 30.738 | 0.00 48.32 | 8 | 6504 | OWO WAT W 162 | 17.100 | 92.730  | 17.506 | 1.00 48.89 | 8 |
| 6463 | OWO WAT W 121 | 39.604 | 81.174  | 29.899 | 1.00 40.72 | 8 | 6505 | OWO WAT W 163 | 54.143 | 65.666  | 53.272 | 1.00 49.78 | 8 |
| 6464 | OWO WAT W 122 | 52.578 | 62.726  | 30.463 | 0.00 55.27 | 8 | 6506 | OWO WAT W 164 | 35.140 | 89.217  | 21.335 | 0.00 49.55 | 8 |
| 6465 | OWO WAT W 123 | 32.284 | 38.992  | 32.423 | 1.00 44.19 | 8 | 6507 | OWO WAT W 165 | 40.864 | 85.144  | 25.201 | 1.00 51.96 | 8 |
| 6466 | OWO WAT W 124 | 54.342 | 58.298  | 13.900 | 1.00 48.84 | 8 | 6508 | OWO WAT W 166 | 0.129  | 71.062  | 53.859 | 1.00 50.46 | 8 |
| 6467 | OWO WAT W 125 | 53.831 | 60.018  | 17.609 | 1.00 53.12 | 8 | 6509 | OWO WAT W 167 | 19.749 | 95.732  | 16.395 | 1.00 54.02 | 8 |
| 6468 | OWO WAT W 126 | 37.548 | 48.910  | 67.790 | 1.00 63.29 | 8 | 6510 | OWO WAT W 168 | 45.089 | 55.696  | 66.763 | 1.00 48.69 | 8 |
| 6469 | OWO WAT W 127 | 16.364 | 67.201  | 64.210 | 1.00 54.77 | 8 | 6511 | OWO WAT W 169 | 29.920 | 93.952  | 27.969 | 1.00 57.82 | 8 |
| 6470 | OWO WAT W 128 | 35.507 | 88.726  | 18.930 | 1.00 44.18 | 8 | 6512 | OWO WAT W 170 | -1.140 | 103.281 | 29.038 | 1.00 59.68 | 8 |
| 6471 | OWO WAT W 129 | 49.585 | 56.011  | 59.240 | 1.00 44.54 | 8 | 6513 | OWO WAT W 171 | 0.493  | 67.332  | 27.261 | 1.00 46.75 | 8 |
| 6472 | OWO WAT W 130 | 13.470 | 54.095  | 28.765 | 1.00 39.17 | 8 | 6514 | OWO WAT W 172 | 11.663 | 49.273  | 52.961 | 1.00 47.65 | 8 |
| 6473 | OWO WAT W 131 | 11.141 | 90.680  | 16.198 | 1.00 49.46 | 8 | 6515 | OWO WAT W 173 | 19.395 | 43.670  | 27.526 | 0.00 52.64 | 8 |
| 6474 | OWO WAT W 132 | -9.184 | 65.150  | 46.616 | 1.00 52.99 | 8 | 6516 | OWO WAT W 174 | 12.558 | 73.429  | 10.221 | 1.00 52.09 | 8 |
| 6475 | OWO WAT W 133 | 44.910 | 67.182  | 7.757  | 1.00 52.67 | 8 | 6517 | OWO WAT W 175 | 47.725 | 72.168  | 25.475 | 1.00 55.03 | 8 |
| 6476 | OWO WAT W 134 | 38.968 | 68.370  | 71.252 | 1.00 37.18 | 8 | 6518 | OWO WAT W 176 | 37.354 | 46.525  | 53.992 | 1.00 62.86 | 8 |
| 6477 | OWO WAT W 135 | 9.962  | 106.661 | 35.598 | 1.00 48.81 | 8 | 6519 | OWO WAT W 177 | 6.566  | 77.689  | 48.060 | 1.00 54.04 | 8 |
| 6478 | OWO WAT W 136 | -0.018 | 83.329  | 37.562 | 1.00 49.93 | 8 | 6520 | OWO WAT W 178 | 27.239 | 80.756  | 54.362 | 1.00 54.49 | 8 |
| 6479 | OWO WAT W 137 | 6.077  | 95.625  | 42.890 | 1.00 41.31 | 8 | 6521 | OWO WAT W 179 | 29.136 | 79.115  | 59.854 | 1.00 51.47 | 8 |

|      |     |     |   |     |        |         |        |      |       |   |
|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| 6522 | OWO | WAT | W | 180 | 51.301 | 65.512  | 30.778 | 1.00 | 58.87 | 8 |
| 6523 | OWO | WAT | W | 181 | 49.729 | 67.077  | 23.232 | 1.00 | 50.64 | 8 |
| 6524 | OWO | WAT | W | 182 | 15.428 | 63.127  | 65.725 | 1.00 | 53.21 | 8 |
| 6525 | OWO | WAT | W | 183 | 28.316 | 47.473  | 59.001 | 1.00 | 52.58 | 8 |
| 6526 | OWO | WAT | W | 184 | 11.167 | 50.777  | 21.789 | 1.00 | 55.21 | 8 |
| 6527 | OWO | WAT | W | 185 | 39.667 | 45.779  | 11.484 | 1.00 | 50.46 | 8 |
| 6528 | OWO | WAT | W | 186 | 9.302  | 78.481  | 48.408 | 1.00 | 50.14 | 8 |
| 6529 | OWO | WAT | W | 187 | -2.511 | 95.777  | 25.082 | 1.00 | 50.26 | 8 |
| 6530 | OWO | WAT | W | 188 | 49.525 | 52.221  | 41.616 | 1.00 | 53.78 | 8 |
| 6531 | OWO | WAT | W | 189 | 33.219 | 90.787  | 32.195 | 1.00 | 53.22 | 8 |
| 6532 | OWO | WAT | W | 190 | 18.629 | 63.971  | 67.355 | 1.00 | 54.97 | 8 |
| 6533 | OWO | WAT | W | 191 | 6.996  | 55.402  | 34.790 | 1.00 | 49.49 | 8 |
| 6534 | OWO | WAT | W | 192 | 50.269 | 70.807  | 60.070 | 1.00 | 54.80 | 8 |
| 6535 | OWO | WAT | W | 193 | -3.948 | 89.479  | 31.518 | 0.00 | 54.80 | 8 |
| 6536 | OWO | WAT | W | 194 | 4.036  | 51.795  | 57.529 | 1.00 | 56.49 | 8 |
| 6537 | OWO | WAT | W | 195 | 15.790 | 48.084  | 23.036 | 1.00 | 52.39 | 8 |
| 6538 | OWO | WAT | W | 196 | 22.577 | 105.708 | 45.361 | 1.00 | 51.14 | 8 |
| 6539 | OWO | WAT | W | 197 | 7.453  | 103.921 | 23.508 | 1.00 | 50.15 | 8 |
| 6540 | OWO | WAT | W | 198 | 37.899 | 80.588  | 45.384 | 1.00 | 52.20 | 8 |
| 6541 | OWO | WAT | W | 199 | 19.774 | 74.879  | 53.890 | 1.00 | 55.07 | 8 |
| 6542 | OWO | WAT | W | 200 | 50.055 | 68.873  | 30.956 | 1.00 | 30.00 | 8 |
| 6543 | OWO | WAT | W | 201 | 53.330 | 63.201  | 30.956 | 1.00 | 37.00 | 8 |
| 6544 | OWO | WAT | W | 202 | 35.086 | 89.130  | 21.284 | 1.00 | 49.00 | 8 |
| 6545 | OWO | WAT | W | 203 | 2.339  | 51.858  | 35.796 | 1.00 | 50.00 | 8 |
| 6546 | OWO | WAT | W | 204 | 19.180 | 43.755  | 27.572 | 1.00 | 50.00 | 8 |
| 6547 | OWO | WAT | W | 205 | 51.693 | 55.504  | 46.921 | 1.00 | 51.00 | 8 |
| 6548 | OWO | WAT | W | 206 | 31.811 | 80.217  | 54.661 | 1.00 | 51.00 | 8 |
| 6549 | OWO | WAT | W | 207 | 11.695 | 77.786  | 12.093 | 1.00 | 51.00 | 8 |
| 6550 | OWO | WAT | W | 208 | 29.940 | 46.996  | 53.693 | 1.00 | 52.00 | 8 |
| 6551 | OWO | WAT | W | 209 | 7.251  | 102.500 | 40.633 | 1.00 | 52.00 | 8 |
| 6552 | OWO | WAT | W | 210 | 23.858 | 91.561  | 17.414 | 1.00 | 52.00 | 8 |
| 6553 | OWO | WAT | W | 211 | 6.783  | 49.832  | 40.633 | 1.00 | 52.00 | 8 |
| 6554 | OWO | WAT | W | 212 | 44.910 | 47.806  | 22.735 | 1.00 | 52.00 | 8 |
| 6555 | OWO | WAT | W | 213 | 36.255 | 46.591  | 10.158 | 1.00 | 52.00 | 8 |
| 6556 | OWO | WAT | W | 214 | 27.601 | 61.581  | 77.880 | 1.00 | 52.00 | 8 |
| 6557 | OWO | WAT | W | 215 | 27.133 | 98.043  | 33.861 | 1.00 | 53.00 | 8 |
| 6558 | OWO | WAT | W | 216 | 18.479 | 55.504  | 45.470 | 1.00 | 53.00 | 8 |
| 6559 | OWO | WAT | W | 217 | 9.122  | 47.401  | 46.438 | 1.00 | 53.00 | 8 |
| 6560 | OWO | WAT | W | 218 | 9.590  | 66.037  | 16.447 | 1.00 | 53.00 | 8 |
| 6561 | OWO | WAT | W | 219 | 13.333 | 91.966  | 46.438 | 1.00 | 53.00 | 8 |

**We claim:**

1. A method of preparing a maltogenic amylase variant having improved anti-staling properties, which method comprises
  - 5 a) subjecting a DNA sequence encoding the maltogenic amylase to random mutagenesis,
  - b) expressing the mutated DNA sequence obtained in step (a) in a host cell, and
  - c) screening for host cells expressing a mutated maltogenic amylase which  
10 shows a higher thermostability, and
  - d) preparing the mutated maltogenic amylase expressed by the host cells.
2. The method of claim 1, wherein the mutated DNA sequence is expressed by transforming a suitable host cell with the mutated DNA sequence and culturing the host cell obtained in step (b) under suitable conditions for expressing the mutated  
15 DNA sequence.
3. A method of producing a variant of a parent maltogenic alpha-amylase, said method comprising
  - a) modeling the parent alpha-amylase on the three-dimensional structure of SEQ ID NO: 1 depicted in the Appendix to produce a three-dimensional  
20 structure of the parent alpha-amylase;
  - b) identifying in the three-dimensional structure obtained in step (a) at least one structural part of the parent wherein an alteration in said structural part is predicted to result in said altered property;
  - c) modifying the sequence of a nucleic acid encoding the parent alpha-  
25 amylase to produce a nucleic acid encoding a deletion, insertion, or substitution of one or more amino acids at a position corresponding to said structural part; and
  - d) expressing the modified nucleic acid in a host cell to produce the variant alpha-amylase,  
30 wherein the variant has alpha-amylase enzymatic activity and has at least one altered property relative to the parent.



4. The method of claim 3, wherein the altered property is pH dependent activity, thermostability, substrate cleavage pattern, specific activity of cleavage, transglycosylation, ability to reduce retrogradation of starch, ability to reduce staling of bread, substrate specificity, substrate binding or calcium binding.

5 5. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:

- 10 a) identifying an amino acid residue which is within 15 Å (in particular 10 Å) from an active site residue of the parent amylase in the three-dimensional structure of said parent, and which is involved in electrostatic or hydrophobic interactions with an active site residue;
- b) substituting said amino acid residue with another amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue, and which can be accommodated in the structure;
- c) optionally repeating steps a) and b) recursively;
- 15 d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b),
- e) preparing the variant resulting from steps a) - d);
- f) testing the pH dependent activity of said variant; and
- g) optionally repeating steps a) - f) recursively; and
- 20 h) selecting a variant having an altered pH dependent activity as compared to the parent amylase.

6. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:

- 25 a) identifying an internal cavity or crevice in the three-dimensional structure of said parent;
- b) substituting an amino acid residue in the neighborhood of the cavity or crevice with another amino acid residue which increases the hydrophobic interaction and/or fills out or reduces the size of the cavity or crevice;
- c) optionally repeating steps a) and b) recursively;
- 30 d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b),
- e) preparing the variant resulting from steps a) - d);
- f) testing the thermostability of said variant; and
- g) optionally repeating steps a) - f) recursively; and
- 35 h) selecting a variant having increased thermostability as compared to the parent amylase.

7. The method of claim 6, wherein the substitution of the amino acid residue results in increasing the hydrophobic interaction, substitution with proline, substitution of histidine with another amino acid, stabilization of calcium binding, introduction of an interdomain disulfide bond, removal of a deamidation site, altering a hydrogen  
5 bond contact, filling in an internal structural cavity with an amino acid with a bulkier side group, introduction of interdomain interactions, altering charge distribution, helix capping, or introduction of a salt bridge.

8. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:

- 10 a) identifying an amino acid residue within 10 Å from a calcium binding site in the three dimensional structure of the amylase;
- b) substituting the amino acid residue with another amino acid residue so as to improve the interaction with the calcium ion;
- c) optionally repeating steps a) and b) recursively;
- 15 d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b),
- e) preparing the variant resulting from steps a) - d);
- f) testing the thermostability of said variant; and
- g) optionally repeating steps a) - f) recursively; and
- 20 h) selecting a variant having increased thermostability as compared to the parent amylase.

9. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:

- 25 a) identifying the substrate binding area in a model of the three-dimensional structure of the parent amylase;
- b) modifying the substrate binding area by an amino acid substitution, deletion or insertion;
- c) optionally repeating step b) recursively;
- d) optionally, making alterations each of which is an insertion, a deletion or a  
30 substitution of an amino acid residue at one or more positions other than b),
- e) preparing the variant resulting from steps a) - d);
- f) testing the substrate-cleavage pattern of the variant.
- g) optionally repeating steps a) - f) recursively; and
- h) selecting a variant having an altered substrate-cleavage pattern as  
35 compared to the parent amylase.

10. A polypeptide which:

- a) has maltogenic amylase activity;
- b) has at least 70 % identity to SEQ ID NO: 1,
- c) has optimum maltogenic amylase activity in the range pH 3.5-7.0 (preferably 4-5.5), and
- 5 d) shows a residual maltogenic amylase activity of at least 25 % after incubation with 1 mM Ca<sup>++</sup> at pH 4.3, 80°C for 15 minutes.

11. A polypeptide which:
- a) has maltogenic alpha-amylase activity;
  - b) has at least 70 % identity to SEQ ID NO: 1; and
  - 10 c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to Q13, I16, D17, N26, N28, P29, A30, S32, Y33, G34, L35, K40, M45, P73, V74, D76, N77, D79, N86, R95, N99, I100, H103, Q119, N120, N131, S141, T142, A148, N152, A163, H169, N171, G172, I174, N176, N187, F188, A192, Q201, N203, H220, N234, G236, Q247, K249, D261, N266, L268, R272, N275, N276, V279, N280, V281, D285, N287, F297, Q299, N305, 15 K316, N320, L321, N327, A341, N342, A348, Q365, N371, N375, M378, G397, A381, F389, N401, A403, K425, N436, S442, N454, N468, N474, S479, A483, A486, V487, S493, T494, S495, A496, S497, A498, Q500, N507, I510, N513, K520, Q526, A555, A564, S573, N575, Q581, S583, F586, K589, N595, G618, 20 N621, Q624, A629, F636, K645, N664 and/or T681; and
  - d) has improved stability compared to the polypeptide of SEQ ID NO: 1.

12. The polypeptide of claim 11, wherein the modification comprises an amino acid modification at a position corresponding to K40, V74, H103, S141, T142, F188, H220, N234, K249, D261, L268, V279, N342, H344, G397, A403, K425, S442, S479, S493, 25 T494, S495, A496, S497, A498, Q500, K520, A555 and/or N595; preferably a substitution corresponding to K40R, V74P, H103Y/V/I/L/F/Y, S141P, T142A, F188I/L, H220Y/L/M, N234P, K249P, D261G, L268P, V279P, N342P, H344E/Q/N/D/Y, G397P, A403P, K425E, S442P, S479P, S493P, T494P, S495P, A496P, S497P, A498P, Q500P, K520R, A555P and/or N595I.

- 30 13. The polypeptide of claim 11 or 12, wherein the modification comprises an amino acid modification at a position corresponding to D17, N28, P29, A30, S32, Y33, G34, R95, H103, N131, H169, I174 and/or Q201 such as to improve calcium coordination, preferably a substitution corresponding to D17Q/E, A30D/M/L/A/V/I/E/Q, S32D/E/N/Q, R95M/L/A/V/I/E/Q, H103Y/N/Q/D/E, N131D, H169N/D/E/Q, I174E/Q, Q201E.

14. The polypeptide of any of claims 11-13, wherein the modification comprises a substitution at a position corresponding to Q13, N26, N77, N86, N99, Q119, N120, N131, N152, N171, N176, N187, Q201, N203, N234, Q247, N266, N275, N276, N280, N287, Q299, N320, N327, N342, Q365, N371, N375, N401, N436, N454, N468, N474, Q500, N507, N513, Q526, N575, Q581, N621, Q624 and/or N664 such as to remove a deamidation site, preferably a substitution corresponding to Q13S/T/A/V/L/I/F/M, N26S/T/A/V/L/I, N77S/T/A/V/L/I, N86S/T/A/V/L/I, N99T/S/V/L, Q119T/S, N120S/T/A/V/L/I, N131S/T/A/V/L/I, N152T/S/V/L, N171Y/D/S/T, N176S/T/A/V/L/I, N187S/T/A/V/L/I, Q201S/T/A/V/L/I/F/M, N203D/S/T/A/V/L/I, N234S/T/A/V/L/I, Q247S/T/A/V/L/I/F/M, N266S/T/A/V/L/I, N275S/T/A/V/L/I, N276S/T/A/V/L/I, N280S/T/A/V/L/I, N287S/T/A/V/L/I, Q299L/T/S, N320S/T/A/V/L/I, N327S/T/A/V/L/I, N342S/T/A/V/L/I, Q365S/T/A/V/L/I, N371S/T/A/V/L/I, N375S/T/A/V/L/I, N401S/T/A/V/L/I, N436S/T/A/V/L/I, N454D/S/T/A/V/L/I, N468D/S/T/A/V/L/I, N474D/S/T/A/V/L/I, Q500S/T/A/V/L/I/F/M, N507S/T/A/V/L/I, N513S/T/A/V/L/I, Q526 D/S/T/A/V/L/I, N575S/T/A/V/L/I, Q581S/T/A/V/L/I/F/M, N621S/T/A/V/L/I, Q624S/T/A/V/L/I/F/M and/or N664D/S/T/A/V/L/I.

15. The polypeptide of any of claims 11-14, wherein the modification comprises a substitution at a position corresponding to I16, L35, M45, P73, D76, D79, A192, I100, A148, A163+G172, L268, V281, D285, L321, F297, N305, K316, S573, A341, M378, A381, F389, A483, A486, I510, A564, F586, K589, F636, K645, A629, and/or T681 such as to improve hydrogen bond contact, preferably a substitution corresponding to I16T/D/N, L35Q, M45K, P73Q, D76E, D79E/Y, A192S/D/N, I100T/S/D/N/E/Q, A148D/N/E/Q/S/T/R/K, A163Y+G172S/D/N, L268R/K, V281/Q, D285R/K, L321Q, F297N/D/Q/E, N305K/R, K316N/D, S573N/D, A341R/K, M378R/K, A381S/D/N, F389Y, A483S/D/N, A486Q/E, I510R/K, A564S/D/N, F586S/D/N, K589S/D/Q/N, F636Y, K645T, A629N/D/E/Q, and/or T681D/N/E/Q/S.

16. The polypeptide of any of claims 11-15, wherein the modification comprises substitutions such as to introduce one or more interdomain disulfide bonds, preferably corresponding to G236C + S583C, G618C + R272C, and/or A348C + V487C.

17. The polypeptide of any of claims 11-16, wherein the substitution at a position corresponding to L51, L75, L78, G88, G91, T94, V114, I125, V126, T134, G157, L217, S235, G236, V254, V279, V281, L286, V289, I290, V308, L321, I325, D326, L343, F349, S353, I359, I405, L448, Q449, L452, I470, G509, V515, S583, G625, L627, L628 and/or A670 so as to fill an internal cavity or crevice, preferably a substitution corresponding to L51W, L75F/Y, L78I, G88A/V/T, G91T/S/V/N, T94V/I/L, V114V/I/L, I125L/M/F/Y/W, V126I/L, T134V/I/L/M/F/Y/W, G157A/V/I/L,

L217V/I/M/F/Y/W, S235I/L/M/F/Y/W, G236A/V/I/L/M/F/Y/W, V254I/L/M/F/Y/W, V279M/I/L/F, V281I/L/M/F/Y/W, L286F, V289I/L/R, I290M/L/F, V308I/L/M/F/Y/W, L321I/M/F/Y/W, I325L/M/F/Y/W, D326E/Q, L343M/F/Y/W, F349W/Y, S353V/I/L, I359L/M/F/Y/W, I405M/L/Y/F/W, L448Y, Q449Y, L452M/Y/F/W, I470M/L/F,  
 5 G509A/V/I/L/M/S/T/D/N, V515I/L, S583V/I/L/V, G625A/V/I/L/M/F/Y/W, L627M/F/Y, L628M/I/F/Y/W, A670V/I/L/M/F/Y/W and/or L217 in combination with L75 (e.g. L217F/Y in combination with L75F/Y).

18. The polypeptide of any of claims 11-17, wherein the modification comprises a substitution at a position corresponding to N106, N320 and Q624 so as to create a  
 10 salt bridge, preferably a substitution corresponding to N106R, N320E/D and/or Q624E.

19. The polypeptide of any of claims 11-18, wherein the modification comprises a substitution at a position corresponding to K244 and/or K316 such as to alter the charge distribution, preferably a substitution corresponding to K244S and/or  
 15 K316G/N/D.

20. The polypeptide of any of claims 11-19, wherein the modification comprises a substitution at a position corresponding to V281 and/or A629 such as to alter the binding site, preferably a substitution corresponding to V281Q and/or A629N/D/E/Q.

21. The polypeptide of any of claims 11-20, wherein the modification comprises  
 20 substitutions such as to alter the interdomain interaction at a position corresponding to F143+F194+L78, A341+A348+L398+I415+T439+L464+L465, L557, S240+L268, Q208+L628, F427+Q500+N507+M508+S573 and/or I510+V620, preferably substitutions corresponding to F143Y+F194Y+L78Y/F/W/E/Q, A341S/D/N+A348V/I/L+L398E/Q/N/D+I415E/Q+T439D/E/Q/N+L464D/E+L465D/E/N/  
 25 Q/R/K, L557Q/E/N/D, S240D/E/N/Q+L268D/E/N/Q/R/K, Q208D/E/Q+L628E/Q/N/D, F427E/Q/R/K/Y+Q500Y+N507Q/E/D+M508K/R/E/Q+S573D/E/N/Q; and/or I510D/E/N/Q/S+V620D/E/N/Q.

22. A polypeptide which:  
 a) has maltogenic alpha-amylase activity;  
 30 b) has at least 70 % identity to SEQ ID NO: 1;  
 c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to D127, V129, F188, A229, Y258, V281, F284, T288, N327, M330, G370, N371, and/or D372; and

d) has altered pH dependent activity as compared to the polypeptide of SEQ ID NO: 1.

23. The polypeptide of claim 22, wherein the modification comprises a substitution corresponding to D127N/L, V129S/T/G/V, F188E/K/H, A229S/T/G/V,  
5 Y258E/D/K/R/F/N, V281L/T, F284K/H/D/E/Y, T288E/K/R, N327D, M330L/F/I/D/E/K, G370N, N371D/E/G/K, and/or D372N/V.

24. A polypeptide which:

- a) has maltogenic alpha-amylase activity;
- b) has at least 70 % identity to SEQ ID NO: 1;
- 10 c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to P191, A192, G193, F194 and/or S195; and
- d) has higher specific amylase activity than the polypeptide of SEQ ID NO: 1.

25. The polypeptide of claim 24, wherein the modification comprises a deletion,  
15 preferably the deletion  $\Delta$  (191-195).

26. The polypeptide of claim 24, wherein the modification comprises insertion, preferably 192-A-193.

27. A polypeptide which:

- a) has maltogenic alpha-amylase activity;
- 20 b) has at least 70 % identity to SEQ ID NO: 1;
- c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to A30, K40, N115, T142, F188, T189, P191, A192, G193, F194, S195, D261, T288, N327, K425, K520 and/or N595; and
- 25 d) has a higher ability than the polypeptide of SEQ ID NO: 1 to reduce retrogradation of starch and/or staling of bread.

28. The polypeptide of claim 27, wherein the modification comprises A30D, K40R, N115D, T142A F188L, T189Y,  $\Delta$  (191-195), D261G, T288P, N327S, K425E, K520R and/or N595I.

29. A process for preparing a dough or a baked product prepared from the dough  
30 which comprises adding the polypeptide of any of claims 10-28, or a variant produced by the method of any of claims 1-8 to the dough in an amount which is effective to retard the staling of the bread.

30. The process of claim 29, wherein the variant is added in an amount of 0.1-5 mg per kg of flour, preferably 0.5-2 mg/kg.
31. A nucleic acid sequence encoding the polypeptide of any of claims 10-27, preferably operably linked to one or more control sequences which direct the expression of the variant in a suitable expression host.
32. A recombinant expression vector comprising the nucleic acid sequence of claim 31, a promoter, and transcriptional and translational stop signals, and preferably further comprising a selectable marker.
33. A transformed host cell comprising the nucleic acid sequence of claim 31 or the vector of claim 32.
34. A method for producing the polypeptide of any of claims 10-27, comprising:
- cultivating the transformed host cell of claim 33 under conditions conducive to expression of the variant; and
  - recovering the variant.

## ABSTRACT

The inventors have modified the amino acid sequence of a maltogenic alpha-amylase to obtain variants with improved properties, based on the three-dimensional structure of the maltogenic alpha-amylase Novamyl. The variants have altered physicochemical properties., e.g. an altered pH optimum, improved thermostability, increased specific activity, an altered cleavage pattern or an increased ability to reduce retrogradation of starch or staling of bread.

Novamyl is a maltogenic alpha-amylase produced by the microorganism *Aspergillus niger*. It is a dimeric protein with a molecular weight of approximately 50,000. The enzyme is highly stable and active in a wide range of pH values (pH 4-10) and temperatures (up to 100°C). It is used in the food industry for the production of malted products and for the improvement of bread staling.



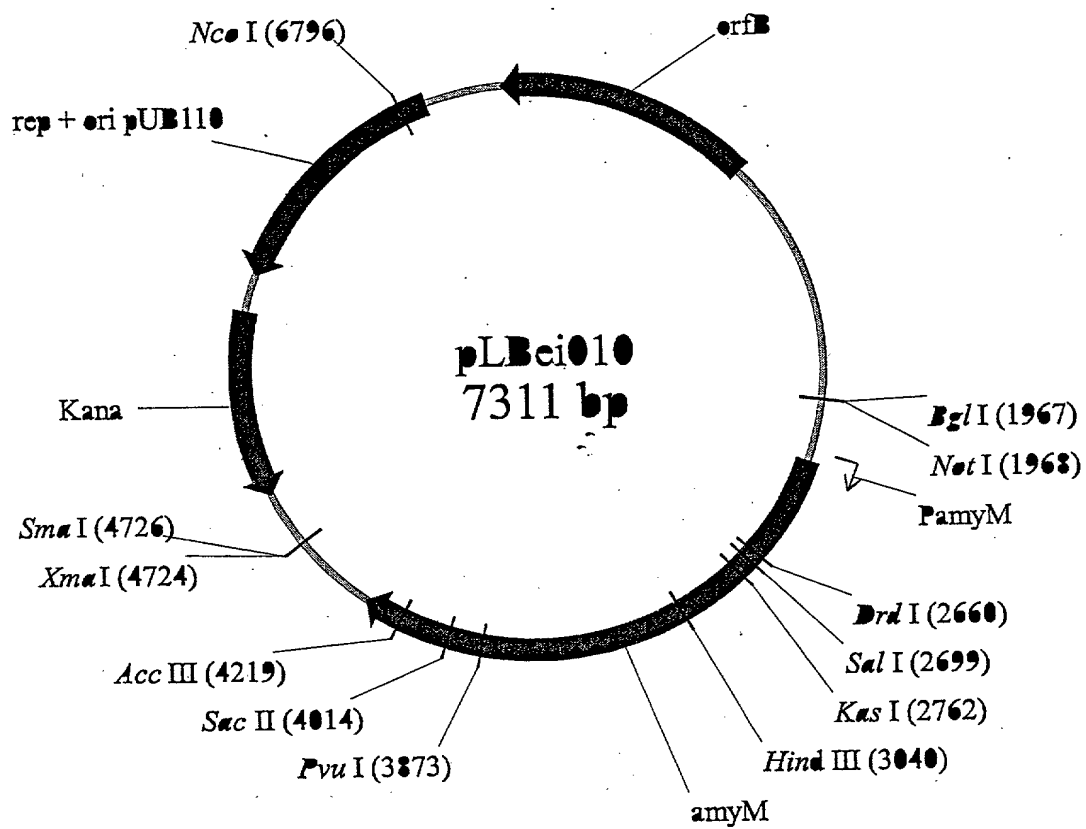


Figure 1

Plasmid pLBei010

As a below named inventor, I hereby declare that:

My residence, post office address and citizenship are as stated below next to my name.

I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:

Maltoqenic Alpha-Amylase Variants

the specification of which (check only one item below):

☐ is attached hereto

☒ was filed as United States application

Application No. 09/386,607

on August 31, 1999

and was amended

on \_\_\_\_\_

☐ was filed as PCT international application

Number \_\_\_\_\_

on \_\_\_\_\_

and was amended under PCT Article 19

on \_\_\_\_\_

I hereby state that I have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

I acknowledge the duty to disclose information which is material to patentability of this application in accordance with Title 37, Code of Federal Regulations, §1.56.

I hereby claim priority benefits under Title 35, United States Code, §119 of any provisional or foreign application(s) for patent or inventor's certificate or of any PCT international application(s) designating at least one country other than the United States of America listed below and have also identified below any foreign application(s) for patent or inventor's certificate or any PCT international application(s) designating at least one country other than the United States of America filed by me on the same subject matter having a filing date before that of the application(s) of which priority is claimed:

PRIOR U.S. PROVISIONAL/FOREIGN/PCT APPLICATION(S) AND ANY PRIORITY CLAIMS UNDER 35 U.S.C. 119:

| COUNTRY<br>(if PCT, indicate "PCT") | APPLICATION NUMBER | DATE OF FILING<br>(day, month, year) | PRIORITY CLAIMED<br>UNDER 35 USC 119                                |
|-------------------------------------|--------------------|--------------------------------------|---|
| Denmark                             | 98/00269           | February 27, 1998                    | <input checked="" type="checkbox"/> YES <input type="checkbox"/> NO |
| U.S.A.                              | 60/077,795         | March 12, 1998                       | <input checked="" type="checkbox"/> YES <input type="checkbox"/> NO |
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|                                     |                    |                                      | <input type="checkbox"/> YES <input type="checkbox"/> NO            |
|                                     |                    |                                      | <input type="checkbox"/> YES <input type="checkbox"/> NO            |

**COMBINED DECLARATION FOR PATENT APPLICATION AND POWER OF ATTORNEY**  
(Includes Reference to PCT International Applications)

Jorney's Docket Number:  
5443.414-US

I hereby claim the benefit under Title 35, United States Code §120 of any United States application(s) or PCT international application(s) designating the United States of America that is/are listed below and, insofar as the subject matter of each of the claims of this applications is not disclosed in that/those prior application(s) in the manner provided by the first paragraph of Title 35, United States Code, §112, I acknowledge the duty to disclose material information as defined in Title 37, Code of Federal Regulations, §1.56(a) which occurred between the filing date of the prior application(s) and the national or PCT international filing date of this application:

**PRIOR U.S. APPLICATIONS OR PCT INTERNATIONAL APPLICATIONS DESIGNATING THE U.S. FOR BENEFIT UNDER 35 U.S.C. 120:**

| U.S. APPLICATIONS       |                   | STATUS (Check one) |         |           |
|-------------------------|-------------------|--------------------|---------|-----------|
| U.S. APPLICATION NUMBER | U.S. FILING DATE  | Patented           | Pending | Abandoned |
| PCT/DK99/00088          | February 26, 1999 |                    | X       |           |
|                         |                   |                    |         |           |
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|                         |                   |                    |         |           |
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**PCT APPLICATIONS DESIGNATING THE U.S.:**

| APPLICATION NO. | FILING DATE | US SERIAL NUMBERS ASSIGNED (if any) |  |  |  |
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|                 |             |                                     |  |  |  |

**POWER OF ATTORNEY:** As a named inventor, I hereby appoint the following attorney(s) and/or agent(s) to prosecute this application and transact all business in the Patent and Trademark Office connected therewith.

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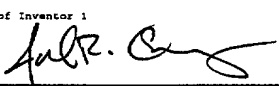

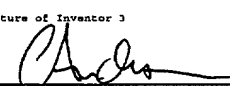


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**COMBINED DECLARATION FOR PAT. APPLICATION AND POWER OF ATTORNEY**  
(Includes Reference to PCT International Applications)

orney's Docket Number:  
5443.414-US

|   |                         |   |                                     |                                     |
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|   | Residence & Citizenship | City  | State or Foreign Country            | Country of Citizenship              |
|   | Post Office Address     | Post Office Address                         | City                                | State & Zip Code/Country            |
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|   | Residence & Citizenship | City  | State or Foreign Country            | Country of Citizenship              |
|   | Post Office Address     | Post Office Address                         | City                                | State & Zip Code/Country            |
| 9 | Full Name of Inventor   | Family Name                                 | First Given Name                    | Second Given Name                   |
|   | Residence & Citizenship | City  | State or Foreign Country            | Country of Citizenship              |
|   | Post Office Address     | Post Office Address                         | City                                | State & Zip Code/Country            |

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under section 1001 of Title 18 of the United States Code, and that such willful false statements may jeopardize the validity of the application or any patent issuing thereon.

|  |   |  |
|--|---|--|
| Signature of Inventor 1<br> | Signature of Inventor 2<br> | Signature of Inventor 3<br> |
| Date<br>28-9-1999  | Date<br>13-9-1999   | Date<br>13-Sep-99  |
| Signature of Inventor 4<br> | Signature of Inventor 5<br> | Signature of Inventor 6  |
| Date<br>24-Sep-99  | Date<br>14/9-1999   | Date   |
| Signature of Inventor 7  | Signature of Inventor 8   | Signature of Inventor 9  |
| Date   | Date  | Date   |

# SEQUENCE LISTING

<110> Cherry, Joel  
Svendsen, Allan  
Andersen, Carsten  
Beier, Lars  
Frandsen, Torben

<120> Maltogenic Alpha-Amylase Variants

<130> 5443.414-US

<140> To Be Assigned

<141> 1999-08-31

<150> DK98/00269

<151> 1998-02-27

<150> 60/077,795

<151> 1998-03-12

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| Arg Asn Asn Ala Ala Ile Gln Tyr Gly Thr Thr Thr Gln Arg Trp Ile |      |
| 400 405 410 415   |      |
| aac aat gat gtt tac att tat gaa cgg aaa ttt ttc aac gat gtc gtg | 1392 |
| Asn Asn Asp Val Tyr Ile Tyr Glu Arg Lys Phe Phe Asn Asp Val Val |      |
| 420 425 430   |      |
| ttg gtg gcc atc aat cga aac acg caa tcc tcc tat tcg att tcc ggt | 1440 |
| Leu Val Ala Ile Asn Arg Asn Thr Gln Ser Ser Tyr Ser Ile Ser Gly |      |
| 435 440 445   |      |
| ttg cag acg gcc ttg cca aat ggc agc tat gcg gat tat ctg tca ggg | 1488 |
| Leu Gln Thr Ala Leu Pro Asn Gly Ser Tyr Ala Asp Tyr Leu Ser Gly |      |
| 450 455 460   |      |
| ctg ttg ggg ggg aac ggg att tcc gtt tcc aat gga agt gtc gct tcg | 1536 |
| Leu Leu Gly Gly Asn Gly Ile Ser Val Ser Asn Gly Ser Val Ala Ser |      |
| 465 470 475   |      |



|   |      |
|---|------|
| ttc acg ctt gcg cct gga gcc gtg tct gtt tgg cag tac agc aca tcc | 1584 |
| Phe Thr Leu Ala Pro Gly Ala Val Ser Val Trp Gln Tyr Ser Thr Ser |      |
| 480 485 490 495   |      |
| gct tca gcg ccg caa atc gga tgc gtt gct cca aat atg ggg att ccg | 1632 |
| Ala Ser Ala Pro Gln Ile Gly Ser Val Ala Pro Asn Met Gly Ile Pro |      |
| 500 505 510   |      |
| ggc aat gtg gtc acg atc gac ggg aaa ggt ttt ggg acg acg cag gga | 1680 |
| Gly Asn Val Val Thr Ile Asp Gly Lys Gly Phe Gly Thr Thr Gln Gly |      |
| 515 520 525   |      |
| acc gtg aca ttt ggc gga gtg aca gcg act gtg aaa tcc tgg aca tcc | 1728 |
| Thr Val Thr Phe Gly Gly Val Thr Ala Thr Val Lys Ser Trp Thr Ser |      |
| 530 535 540   |      |
| aat cgg att gaa gtg tac gtt ccc aac atg gcc gcc ggg ctg acc gat | 1776 |
| Asn Arg Ile Glu Val Tyr Val Pro Asn Met Ala Ala Gly Leu Thr Asp |      |
| 545 550 555   |      |
| gtg aaa gtc acc gcg ggt gga gtt tcc agc aat ctg tat tct tac aat | 1824 |
| Val Lys Val Thr Ala Gly Gly Val Ser Ser Asn Leu Tyr Ser Tyr Asn |      |
| 560 565 570 575   |      |
| att ttg agt gga acg cag aca tgc gtt gtg ttt act gtg aaa agt gcg | 1872 |
| Ile Leu Ser Gly Thr Gln Thr Ser Val Val Phe Thr Val Lys Ser Ala |      |
| 580 585 590   |      |
| cct ccg acc aac ctg ggg gat aag att tac ctg acg ggc aac ata ccg | 1920 |
| Pro Pro Thr Asn Leu Gly Asp Lys Ile Tyr Leu Thr Gly Asn Ile Pro |      |
| 595 600 605   |      |
| gaa ttg ggg aat tgg agc acg gat acg agc gga gcc gtt aac aat gcg | 1968 |
| Glu Leu Gly Asn Trp Ser Thr Asp Thr Ser Gly Ala Val Asn Asn Ala |      |
| 610 615 620   |      |
| caa ggg ccc ctg ctc gcg ccc aat tat ccg gat tgg ttt tat gta ttc | 2016 |
| Gln Gly Pro Leu Leu Ala Pro Asn Tyr Pro Asp Trp Phe Tyr Val Phe |      |
| 625 630 635   |      |
| agc gtt cca gca gga aag acg att caa ttc aag ttc ttc atc aag cgt | 2064 |
| Ser Val Pro Ala Gly Lys Thr Ile Gln Phe Lys Phe Phe Ile Lys Arg |      |
| 640 645 650 655   |      |

gcg gat gga acg att caa tgg gag aat ggt tgg aac cac gtg gcc aca 2112  
 Ala Asp Gly Thr Ile Gln Trp Glu Asn Gly Ser Asn His Val Ala Thr  
                   660                  665                  670

act ccc acg ggt gca acc ggt aac att act gtt acg tgg caa aac tag 2160  
 Thr Pro Thr Gly Ala Thr Gly Asn Ile Thr Val Thr Trp Gln Asn  
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Gly Leu Leu Phe Ser Gly Ser Leu Pro Tyr Asn Pro Asn Ala Ala Glu  
                   20                              25                              30

Ala Ser Ser Ser Ala Ser Val Lys Gly Asp Val Ile Tyr Gln Ile Ile  
           35                              40                              45

Ile Asp Arg Phe Tyr Asp Gly Asp Thr Thr Asn Asn Asn Pro Ala Lys  
       50                              55                              60

Ser Tyr Gly Leu Tyr Asp Pro Thr Lys Ser Lys Trp Lys Met Tyr Trp  
       65                              70                              75                              80

Gly Gly Asp Leu Glu Gly Val Arg Gln Lys Leu Pro Tyr Leu Lys Gln  
                   85                              90                              95

Leu Gly Val Thr Thr Ile Trp Leu Ser Pro Val Leu Asp Asn Leu Asp  
           100                              105                              110

Thr Leu Ala Gly Thr Asp Asn Thr Gly Tyr His Gly Tyr Trp Thr Arg

115

120

125

Asp Phe Lys Gln Ile Glu Glu His Phe Gly Asn Trp Thr Thr Phe Asp  
130 135 140

Thr Leu Val Asn Asp Ala His Gln Asn Gly Ile Lys Val Ile Val Asp  
145 150 155 160

Phe Val Pro Asn His Ser Thr Pro Phe Lys Ala Asn Asp Ser Thr Phe  
165 170 175

Ala Glu Gly Gly Ala Leu Tyr Asn Asn Gly Thr Tyr Met Gly Asn Tyr  
180 185 190

Phe Asp Asp Ala Thr Lys Gly Tyr Phe His His Asn Gly Asp Ile Ser  
195 200 205

Asn Trp Asp Asp Arg Tyr Glu Ala Gln Trp Lys Asn Phe Thr Asp Pro  
210 215 220

Ala Gly Phe Ser Leu Ala Asp Leu Ser Gln Glu Asn Gly Thr Ile Ala  
225 230 235 240

Gln Tyr Leu Thr Asp Ala Ala Val Gln Leu Val Ala His Gly Ala Asp  
245 250 255

Gly Leu Arg Ile Asp Ala Val Lys His Phe Asn Ser Gly Phe Ser Lys  
260 265 270

Ser Leu Ala Asp Lys Leu Tyr Gln Lys Lys Asp Ile Phe Leu Val Gly  
275 280 285

Glu Trp Tyr Gly Asp Asp Pro Gly Thr Ala Asn His Leu Glu Lys Val  
290 295 300

Arg Tyr Ala Asn Asn Ser Gly Val Asn Val Leu Asp Phe Asp Leu Asn  
305 310 315 320

Thr Val Ile Arg Asn Val Phe Gly Thr Phe Thr Gln Thr Met Tyr Asp  
325 330 335

Leu Asn Asn Met Val Asn Gln Thr Gly Asn Glu Tyr Lys Tyr Lys Glu  
340 345 350

Asn Leu Ile Thr Phe Ile Asp Asn His Asp Met Ser Arg Phe Leu Ser  
355 360 365

Val Asn Ser Asn Lys Ala Asn Leu His Gln Ala Leu Ala Phe Ile Leu  
370 375 380

Thr Ser Arg Gly Thr Pro Ser Ile Tyr Tyr Gly Thr Glu Gln Tyr Met  
385 390 395 400

Ala Gly Gly Asn Asp Pro Tyr Asn Arg Gly Met Met Pro Ala Phe Asp  
405 410 415

Thr Thr Thr Thr Ala Phe Lys Glu Val Ser Thr Leu Ala Gly Leu Arg  
420 425 430

Arg Asn Asn Ala Ala Ile Gln Tyr Gly Thr Thr Thr Gln Arg Trp Ile  
435 440 445

Asn Asn Asp Val Tyr Ile Tyr Glu Arg Lys Phe Phe Asn Asp Val Val  
450 455 460

Leu Val Ala Ile Asn Arg Asn Thr Gln Ser Ser Tyr Ser Ile Ser Gly  
465 470 475 480

Leu Gln Thr Ala Leu Pro Asn Gly Ser Tyr Ala Asp Tyr Leu Ser Gly  
485 490 495

Leu Leu Gly Gly Asn Gly Ile Ser Val Ser Asn Gly Ser Val Ala Ser  
500 505 510

Phe Thr Leu Ala Pro Gly Ala Val Ser Val Trp Gln Tyr Ser Thr Ser  
515 520 525

Ala Ser Ala Pro Gln Ile Gly Ser Val Ala Pro Asn Met Gly Ile Pro  
530 535 540

Gly Asn Val Val Thr Ile Asp Gly Lys Gly Phe Gly Thr Thr Gln Gly  
545 550 555 560

Thr Val Thr Phe Gly Gly Val Thr Ala Thr Val Lys Ser Trp Thr Ser  
565 570 575

Asn Arg Ile Glu Val Tyr Val Pro Asn Met Ala Ala Gly Leu Thr Asp  
580 585 590

Val Lys Val Thr Ala Gly Gly Val Ser Ser Asn Leu Tyr Ser Tyr Asn  
595 600 605

Ile Leu Ser Gly Thr Gln Thr Ser Val Val Phe Thr Val Lys Ser Ala  
610 615 620

Pro Pro Thr Asn Leu Gly Asp Lys Ile Tyr Leu Thr Gly Asn Ile Pro  
625 630 635 640

Glu Leu Gly Asn Trp Ser Thr Asp Thr Ser Gly Ala Val Asn Asn Ala  
645 650 655

Gln Gly Pro Leu Leu Ala Pro Asn Tyr Pro Asp Trp Phe Tyr Val Phe  
660 665 670

Ser Val Pro Ala Gly Lys Thr Ile Gln Phe Lys Phe Phe Ile Lys Arg  
675 680 685

Ala Asp Gly Thr Ile Gln Trp Glu Asn Gly Ser Asn His Val Ala Thr  
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34

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<212> DNA

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20

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